PB81-200529

Guideline for Applying the Airshed Model to Urban Areas

(U.S.) Environmental Protection Agency
Research Triangle Park, NC

Oct 80

U.S. Department of Commerce
National Technical Information Service
NTIS

United States
Environmental Protection
Agency

Office of Air Quality
Planning and Standards
Research Triangle Park NC 27711

EPA-450/4-80-020
October 1980

Air

PB81-200529

EPA

Guideline For Applying The Airshed Model To Urban Areas

PRODUCT OF:
NATIONAL TECHNICAL
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U.S. DEPARTMENT OF COMMERCE
SPRINGFIELD, VA. 22161

TECHNICAL REPORT DATA
(Please read Instructions on the reverse before completing)

1. REPORT NO. EPA 450/4-80-020	2.	3. RECIPIENT'S ACCESSION NO. PB81 200529
4. TITLE AND SUBTITLE Guideline for Applying the Airshed Model to Urban Areas		5. REPORT DATE October 1980
		6. PERFORMING ORGANIZATION CODE
7. AUTHOR(S)		8. PERFORMING ORGANIZATION REPORT NO.
9. PERFORMING ORGANIZATION NAME AND ADDRESS Monitoring and Data Analysis Division Office of Air Quality Planning and Standards Research Triangle Park, North Carolina 27711		10. PROGRAM ELEMENT NO.
		11. CONTRACT/GRANT NO.
12. SPONSORING AGENCY NAME AND ADDRESS Same.		13. TYPE OF REPORT AND PERIOD COVERED
		14. SPONSORING AGENCY CODE
15. SUPPLEMENTARY NOTES		

16. ABSTRACT

Guidance is provided to potential model users on the capabilities of the Airshed Model, its data requirements, and its application to control strategy analyses. The Airshed Model is an urban-scale, grid-based, photochemical dispersion model. Its greatest utility lies in studying the relationship of emissions of volatile organic compounds and nitrogen oxides to ambient ozone levels observed in major metropolitan areas. However, the model may be used to estimate ambient short-term concentrations of nitrogen dioxide and carbon monoxide as well. The guideline should enable air pollution control agencies and others to carry out the planning activities and to evaluate the level of resources needed to apply the model.

17. KEY WORDS AND DOCUMENT ANALYSIS

a. DESCRIPTORS	b. IDENTIFIERS/OPEN ENDED TERMS	c. COSATI Field/Group
Air Pollution Atmospheric Models	Photochemical Model Ozone	

18. DISTRIBUTION STATEMENT Release Unlimited	19. SECURITY CLASS *(This Report)* Unclassified	21. NO. OF PAGES
	20. SECURITY CLASS *(This page)* Unclassified	22. PRICE

EPA Form 2220-1 (9-73)

EPA-450/4-80-020

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U.S. ENVIRONMENTAL PROTECTION AGENCY
Office of Air, Noise, and Radiation
Office of Air Quality Planning and Standards
Monitoring and Data Analysis Division
Research Triangle Park, North Carolina 27711

October 1980

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Publication No. EPA-450/4-80-020

ACKNOWLEDGEMENTS

This guideline was prepared by David E. Layland of the Source Receptor Analysis Branch of the Monitoring and Data Analysis Division of the Office of Air Quality Planning and Standards. John Summerhays, also of the Source Receptor Analysis Branch, made important contributions to the guideline. E. L. Martinez and Dr. Henry S. Cole provided additional assistance. Guidance and direction were given by Joseph A. Tikvart and David H. Barrett. Steven D. Reynolds, Thomas W. Tesche, and Lawrence E. Reid of Systems Applications, Incorporated provided various materials which were adapted for inclusion in the guideline. Appreciation is extended to Zada Nelson for her care and patience in preparing the manuscript.

FOREWORD

High ozone levels are one of the most pervasive air pollution problems facing our nation's cities. While the planning and analysis tools available to grapple with the problem have been less than ideal, the costs associated with the types of control measures necessary to alleviate the problem are high.

The need for credible modeling techniques for evaluating the relationship between emission reductions and ozone levels on an urban scale is widely recognized. A credible technique should possess at least two basic attributes. First, it should account for all significant physical and chemical processes and second, it should be capable of being verified.

Empirical techniques have been proposed and used for developing State Implementation Plans called for by the Clean Air Act. Unfortunately, empirical techniques have not fully satisfied the criteria of technical rigor and verifiability. Photochemical grid models on the other hand meet both of these criteria. However, the benefits of using such models are achieved at appreciable cost in terms of data requirements.

The physical and chemical processes which lead to high observed ozone levels are complex. The relationship between precursor emissions and ozone air quality is time and space dependent. Among the major factors affecting the generation of ozone are:

- the quantity and the spatial and temporal distribution of emissions of nitrogen oxides and volatile organics
- the chemical composition of the volatile organics emitted
- the chemical reactions among ozone, organics, and nitrogen oxides

- the spatial and temporal nature of the wind field
- the stability of the atmosphere and the dynamics of the mixed layer
- the intensity and diurnal variation of solar radiation
- the transport of ozone and its precursors into the urban area from aloft and immediately upwind
- the loss of ozone and precursors by surface uptake

The Environmental Sciences Research Laboratory of the Office of Research and Development, U. S. Environmental Protection Agency, has supported a multi-year research effort by Systems Applications, Inc. (SAI) of San Rafael, California. This research has led to the development of the Airshed Model. Initial model development efforts and applications to the Los Angeles area are fully described in a 15-volume series of reports by Roth, et al., (1971) and Reynolds, et al., (1973a). These reports are summarized in three papers by Reynolds, et al., (1973b, 1974) and Roth, et al., (1974). Evaluation of the model's predictions and its components at that time showed that improved treatments of some physical and chemical processes were necessary. As a result, another series of research efforts was carried out to improve the model. These efforts are described in a seven-volume series of reports by Jerskey and Seinfeld (1976), Jerskey, et al., (1976), Killus, et al., (1977), Lamb (1976), Lamb, et al., (1977), Liu, et al., (1976a), and Reynolds, et al., (1976) and in papers by

Lamb, Chen, and Seinfeld (1975), Liu and Seinfeld (1975), Liu, Whitney, and Roth (1976), and Reynolds (1977).

Previous versions of the Airshed Model have been successfully applied in Los Angeles, Denver, and Sacramento. These applications are reported in Reynolds, et al., (1979), Reynolds, et al., (1978), and Anderson, et al., (1977). Future applications are planned for Tulsa, Philadelphia, Washington, D. C., Baltimore, New York City, and Boston.

Although this guideline is written in terms of applying the Airshed Model, the same general principles apply to the application of any photochemical grid model. Mention of the Airshed Model by name does not constitute formal endorsement of or preference for this model at this time.

The purpose of this guideline is to familiarize air pollution control agencies and others with the Airshed Model and its potential for use in State Implementation Plan (SIP) development and for evaluating alternative strategies for the control of photochemical oxidants. This is not a how-to document nor a formal planning document. Rather, it is one which attempts to outline what tasks are involved in using the Airshed Model. With this information it is hoped that control agencies contemplating a photochemical model application will be able to effectively plan for such a project. Planning considerations will be unique for each individual application. For example, the extent to which in-house versus contract resources are used must be considered on a case by case basis. This document only describes the kinds of tasks involved and the overall level of resources required for an Airshed Model application.

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Appendix. Technical Description of the Airshed Model A-1

CHAPTER I. PRINCIPLES OF THE AIRSHED MODEL

A. MODEL CONCEPTS AND MECHANICS

The Airshed Model is a photochemical dispersion model designed to simulate the concentrations of ozone and its precursors (nitrogen oxides and organics*) as they evolve during a day's episode. This involves using a detailed set of meteorological and emissions data in order to simulate the emissions of precursors, atmospheric dispersion, and the chemical reactions that generate ozone.

The basis of the mathematics for simulating concentrations of ozone and precursors is the conservation of mass. The major processes which cause changes in the amount of mass in a given air parcel are emissions, advection and dispersion of mass into and out of the parcel, and chemical changes in the composition of the parcel. Thus photochemical dispersion models are based on solving the following equation (restated in terms of concentrations:

$$\text{Concentration} = \text{initial concentration} + \left(\frac{\text{(mass in)-(mass out) due to advection and dispersion}}{\text{parcel volume}}\right) + \left(\frac{\text{mass of emissions}}{\text{parcel volume}}\right) + \text{change in concentration due to chemical transformation} \qquad (1)$$

In the Airshed Model, the urban area is divided into a three dimensional grid system for which solutions of Equation (1) are derived individually for each grid cell. This process is illustrated in Figure I-1.

The first term in Equation (1) is "concentration." The purpose of running the Airshed Model is to estimate the concentration of ozone

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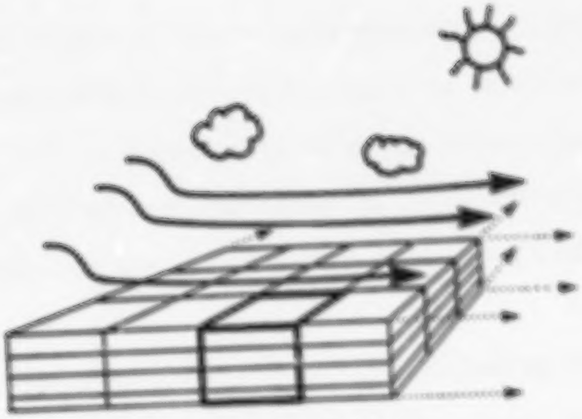
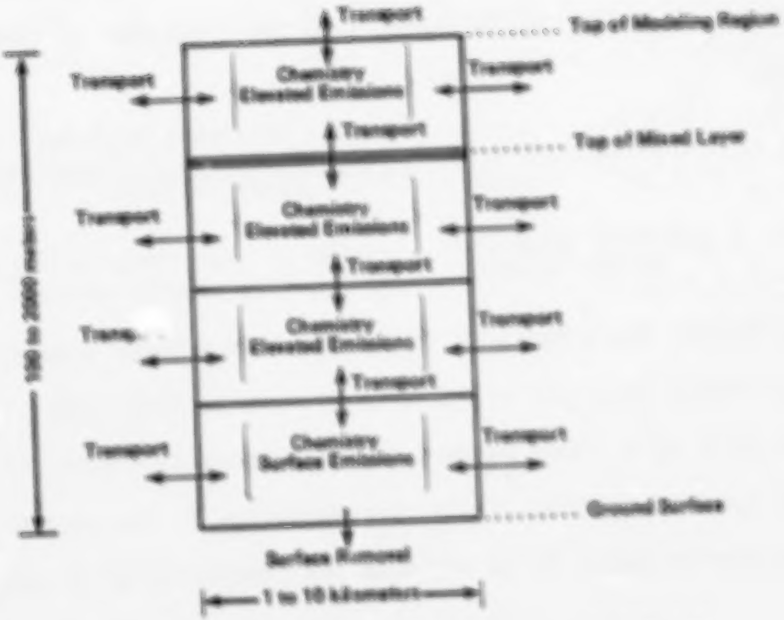
*The term "organics" includes both simple hydrocarbons and oxygenated organics. However, the term organics and the term hydrocarbons are used interchangeably.



(a) SPECIFICATION OF THE GRID


Transport
Top of Modeling Region
Transport
Chemistry
Elevated Emissions
Transport
Transport
Top of Mixed Layer
Transport
Chemistry
Elevated Emissions
Transport
Transport
Trans.
Chemistry
Elevated Emissions
Transport
Transport
Transport
Chemistry
Surface Emissions
Transport
Ground Surface
Surface Removal
1 to 10 kilometers
100 to 2000 meters

(b) ATMOSPHERIC PROCESSES TREATED IN A COLUMN OF GRID CELLS.

Figure I-1. Schematic illustration of the grid used and atmospheric processes treated in the airshed model (adapted from Reynolds, Tesche, and Reid, 1978).

in each grid cell for a particular day. This requires solving Equation (1) not only for ozone but also for NO, NO_2 and five classes of organic compounds. These five classes of organics roughly correspond to paraffins, olefins, aromatics, aldehydes and ethylene. The nature of the five classes and the rationale for making the distinction is discussed later in this chapter. Also discussed later are several other species indirectly affecting ozone production which may optionally be simulated in the Airshed Model. Thus a simulation using the Airshed Model involves calculating the concentrations of each major species in each grid cell for each hour being simulated. For example, a typical model run may simulate 14 hours (5 a.m. to 7 p.m.) using a grid system of 1200 grid cells (15 cells east-west, 20 cells north-south, and 4 cells high) or more. Consequently, the Airshed Model makes a large number of calculations in simulating the formation of ozone on any given day.

The next term in Equation (1) is the initial concentration. The equation suggests that the concentration at the end of a time step equals the concentration at the beginning of the time step plus the changes in concentration (due to advection, dispersion, emissions, and chemistry) that occur during the time step. The length of a time step is usually six minutes or less. The user must supply the initial concentrations for the first time step of the simulation. The concentrations calculated at the end of the first time step are then used as the initial concentrations at the second time step. This process continues until the entire desired time period has been simulated.

A typical time for starting simulations is 5 a.m. This is prior to the morning rush hour and so concentrations are still fairly low. This makes the model estimates less sensitive to initial concentration measurements and more sensitive to the chemical and physical processes being simulated during the day. Thus, the Airshed Model requires a concentration at the beginning of the simulation, i.e., initial conditions, for each species (O_3, NO, NO_2, five classes of organics and any optional species) for each grid cell.

The next term in Equation (1) represents the effects of winds and turbulent mixing. From the perspective of an individual grid cell, the wind portion of this term is based on the difference between the pollutant concentration transported in from upwind cells and the pollutant concentration being transported out of the cell. The dispersion portion of this term is based on the concentration gradients between the cell and each of the six neighboring cells (above, below, and four sides). From a broader perspective, it is also necessary to be able to estimate the mass which is advected and diffused into the modeling region as a whole. Thus, an input requirement of the Airshed Model is a set of concentrations at the boundary of the modeling region, i.e., boundary conditions. More specifically, the Airshed Model requires that estimates of the concentrations be input for all species (i.e., O_3, NO, NO_2, five classes of organics and any optional species) for each hour simulated along the sides and at the top of the modeling region.

It is generally desirable to define the modeling region such that the upwind boundary is, in fact, upwind of the city, in order that the boundary concentrations are relatively low. However, in many parts of the United States, substantial concentrations of ozone and other pollutants are transported into a city from long distances upwind. This pollutant transport is reflected in the boundary concentrations used in the simulation. Thus, it is often important to obtain an accurate estimate of boundary concentrations.

The third term on the right side of Equation (1) accounts for pollutant emissions. This term is quite important, since the purpose of using the Airshed Model is to determine the relationship between emissions of hydrocarbons and NO_x and the resulting concentrations of ozone. The model requires the emissions of these species to be specified for each grid cell for each hour that is simulated. Most of the emissions are added to the lowest grid cell in the respective column of cells. However, the Airshed Model also has the capability of adding emissions from elevated point sources to elevated grid cells. Thus, the Airshed Model introduces the emissions at the height at which they are actually found.

The final term in Equation (1) accounts for the effects of chemical transformations. This term expresses the changes in chemical composition of the atmosphere that occur as hydrocarbons and NO_x react in the presence of sunlight to form ozone. This is one of the most complex components of the Airshed Model. Fortunately, the chemistry of the Airshed Model is fully contained within the model, so the user is not required to supply any information about atmospheric chemistry.

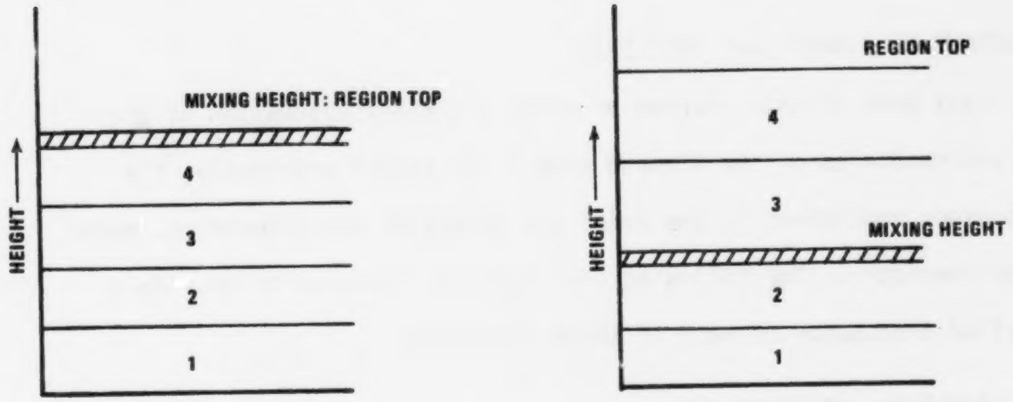
The Airshed Model also has the option for simulating the concentration of carbon monoxide. Since CO is relatively nonreactive, simulation of CO concentrations is useful for checking the accuracy of the model's treatment of advection and dispersion.

It should be clear from the above discussion that the Airshed Model is substantially different from the Gaussian dispersion models typically used for inert pollutants. First, the Airshed Model does not assume steady state conditions, since ozone concentrations are a function of the complete meteorological and chemical history of the air mass. Unlike most inert pollutant model applications, the Airshed Model considers the chemical interactions of emissions from throughout the urban area. Also, the Airshed Model does not use the empirically derived dispersion coefficients (i.e., sigmas) inherent in the Gaussian formulation. Instead, the Airshed Model uses eddy diffusivity coefficients to estimate dispersion.

The above discussion has outlined the concepts by which the major physical and chemical processes are considered in the Airshed Model. In order to discuss the mechanics of the Airshed Model, however, it is necessary to discuss gridding. As mentioned previously, a typical application of the Airshed Model might use a grid system of 15 cells by 20 cells horizontally by 4 cells vertically. Each cell has constant horizontal dimensions, say 4 kilometers by 4 kilometers. On the other hand, the vertical dimensions of the cells vary in time according to changes in the mixing height. The user determines how many cells will be used below the mixing height. In this way the mixed layer is divided into several cells of equal dimension. The vertical dimensions of the cells typically range from 25 to 500 meters.

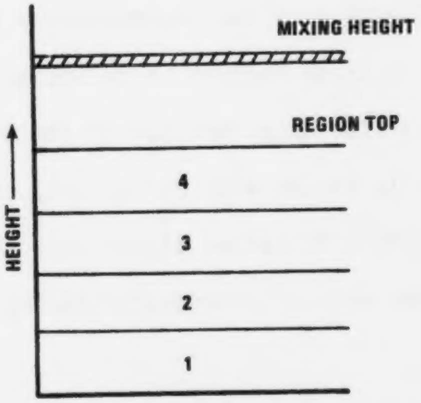
An important option in the Airshed Model is to use cells above the mixed layer. These cells become significant when the mixing height rises, thereby entraining pollutants from these cells into the mixed layer. This process, known as fumigation, is a frequent occurrence in the late morning hours as the mixing height rises rapidly. Early morning emissions from elevated point sources become trapped in these cells and are then mixed to the ground later in the day.

Figures I-2(a) through (c) show the various possibilities for specifying the vertical dimensions of cells. Figure I-2(a) and I-2(b) show the options of simulating the mixed layer with and without also simulating an elevated inversion layer. Figure I-2(c) shows that a third option of the Airshed Model is to have the top of the modeling region below the mixing height. The purpose of this option is to reduce the vertical dimensions of


MIXING HEIGHT: REGION TOP
4
3
2
1
HEIGHT
REGION TOP
4
3
MIXING HEIGHT
2
1
HEIGHT

(a) MODELING REGION IS THE SAME HEIGHT AS MIXED LAYER

(b) MODELING REGION INCLUDES CELLS ABOVE MIXED LAYER


MIXING HEIGHT
REGION TOP
4
3
2
1
HEIGHT

(c) MODELING REGION DOES NOT INCLUDE THE ENTIRE MIXED LAYER

Figure I-2. Several possible options for vertical gridding.

the cells and thus improve the vertical resolution. However, this option has the disadvantage that the mixing height is not within the modeling region making it difficult to properly simulate the effect of a lid on the vertical flow of pollutants.

B. TREATMENT OF SIGNIFICANT PROCESSES

The first part of this chapter provided a general discussion of the concepts and mechanics of the Airshed Model. As stated previously, the major processes considered in the model are advection and dispersion, emissions, and chemistry. The following discussion is intended to provide a more detailed discussion of each of these processes.

1. Advection and Dispersion

Since the Airshed Model simulates concentrations in fixed grid cells, advection and dispersion are simulated by transferring appropriate amounts of pollutants from one cell to another. Pollutants are transferred horizontally from one cell to the next as a function of the concentration and the speed of the wind. The flux of material due to these factors is called advection. Pollutants are transferred between two cells also as a function of the difference between the concentrations in the two cells and an eddy diffusivity coefficient. The flux of material due to these factors is called dispersion. The eddy diffusivity coefficient expresses the rate of atmospheric mixing caused by turbulent eddies.

The Airshed Model also simulates vertical advective transfer. Vertical transfer arises primarily from two sources: (1) balancing the effect of convergence and/or divergence of horizontal winds in order to achieve a proper mass balance of air, and (2) accounting for changes in cell height as the mixing height changes. The first source of vertical transfer must be considered in preparing the wind data for use in the model. For example, if the horizontal winds are converging in a cell, the wind field used in the model must have a sufficient vertical component to prevent an artificial accumulation of pollutants in the cell. The second source of vertical transfer is an artificial one arising from the mechanics of the simulation program. As the cell height increases, material located at a given height may be transferred from one cell to another without actually changing its relative vertical position.

The Airshed Model has differences in its treatments of vertical and horizontal dispersion. Because horizontal dispersion is generally less important than advection, the Airshed Model uses a single horizontal eddy diffusivity coefficient. However, vertical eddy diffusivity coefficients are individually calculated for each cell and each time period as a function of atmospheric stability and surface roughness.

2. Emissions

The treatment of emissions is straightforward conceptually: the emissions into a cell are added uniformly throughout the cell. Thus, the change in concentration due to emissions simply equals the mass added divided by the volume of the cell. Ground-level emissions are added into the lowest level cell. Elevated emissions are added into upper level cells. This requires that certain stack parameters be input for the major point sources. The stack parameters are used along with the wind speed to estimate an effective plume height for each major point source. The emissions are then added uniformly throughout the (upper level) cell which is calculated to receive the plume.

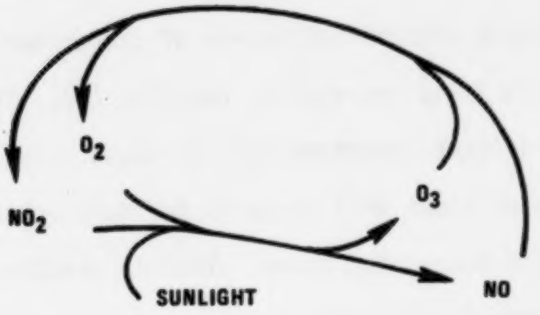
The Airshed Model is designed to treat emissions of eight pollutants: NO, NO_2 five classes of organics and CO. NO_x emissions must therefore be divided into emissions of NO and NO_2 and organics must be divided into emissions of five organics classes. These classes are discussed in Section 3.

A point of comparison between the Airshed Model and Gaussian dispersion models is the treatment of plume rise. Like most inert pollutant dispersion models, the Airshed Model uses the Briggs (1971) formulae to estimate plume rise. However, unlike most Gaussian models, the Airshed Model is capable of simulating emissions that rise above the mixed layer. Inert pollutant models generally disregard any emissions in plumes that rise above the mixing height. Although the Airshed Model also disregards any emissions in plumes that rise above the top of the modeling region, the modeling region in the Airshed Model can extend above the mixing height. It is thus possible to simulate plumes that rise into an inversion layer between the mixing height and the top of the modeling region.

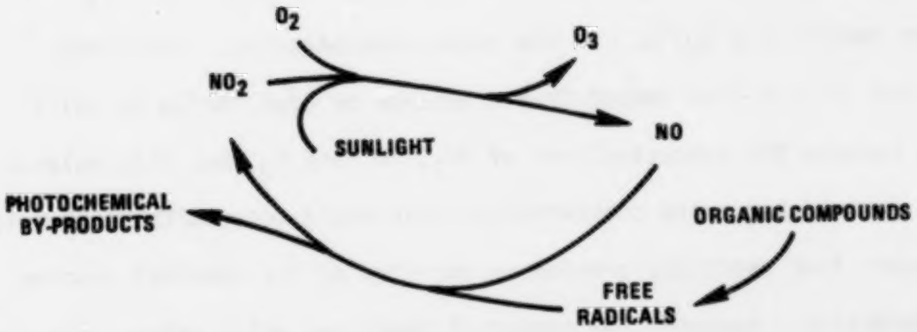
3. Chemistry

As mentioned previously, the chemical mechanism is one of the most complex components of the Airshed Model. The chemistry of ozone production has been the subject of intensive study for well over a decade, and yet there is surprisingly little agreement on the list of reactions to use in simulating ozone photochemistry. Thus, this discussion will only provide a general outline of the photochemistry of ozone production. The discussion will then outline the major distinguishing features of the chemical mechanism used in the Airshed Model.

The general process by which tropospheric ozone is formed is illustrated in Figure I-3. Figure I-3(a) shows the NO_2-NO-O_3 cycle. These reactions may be written as chemical equations:


O$_2$
O$_3$
NO$_2$
SUNLIGHT
NO

(a) THE NO_2-NO-O_3 CYCLE


O$_2$
O$_3$
NO$_2$
SUNLIGHT
NO
PHOTOCHEMICAL BY-PRODUCTS
ORGANIC COMPOUNDS
FREE RADICALS

(b) ORGANIC OXIDATION OF NO TO NO_2 WITH OZONE BUILDUP

Figure I-3. Photochemical production of oxidants.

a. NO_2 + sunlight → NO + O

b. $O + O_2 \rightarrow O_3$

c. $O_3 + NO \rightarrow NO_2 + O_2$

Ozone is not emitted in any measurable quantity, and in fact, reactions (a) and (b) represent the only significant source of tropospheric ozone. However, these reactions are fully reversed by reaction (c). Thus, NO_x by itself will not cause significant concentrations of ozone. The only way significant concentrations of ozone will occur is for some other species to oxidize NO to NO_2 without destroying ozone. This is exactly what is shown in Figure I-3(b). This may be written as:

d. Organic radicals + NO → NO_2 + miscellaneous products

The net result of reactions (a), (b), and (d), then, is a recycling of NO_2/NO, a modification of the organic species, and the generation of an excess O_3 molecule. That is, organic species permit the ozone formation step while bypassing the ozone destruction step of the $NO_2 - NO - O_3$ cycle. The result is a buildup of the ozone concentration. Reactions (a), (b), and (c) are fast enough that a balance or equilibrium is still maintained between the concentrations of NO_2, NO, and O_3, but this balance involves a much higher ozone concentration than would occur without organics.

The above four reactions provide an overview of the chemical process of ozone formation. However, the number of reactions which affect this process is far larger. In fact, the number of reactions involved is too large for all the reactions to be included in photochemical models. Thus the chemical reactions simulated in these models are a simplified representation of the innumerable reactions that actually occur.

It is more difficult to represent the various reactions of organics than it is to represent the reactions of NO_x. There is substantial agreement on about 10 to 15 NO_x reactions as being the most significant reactions for describing the fate of NO_x. However, there is relatively little agreement as to how best to represent organic reactions. This is primarily due to the almost infinite number of species and reactions that occur. In tracing the entire path of decomposition of just one organic species, it is possible to list over 100 reactions of that species and the products of its decomposition. Moreover, urban emissions include a wide variety of organic species. Therefore, a simplified representation of all these reactions is needed.

The typical means of representing significant organic reactions is to utilize a small number of reactions for about three to five categories of organics. For example, the Livermore Regional Air Quality (LIRAQ) model developed by the Lawrence Livermore Laboratory at Livermore, California, (MacCracken and Sauter (1975), MacCracken et al., (1978)) uses three categories of organics roughly described as olefins, paraffins, and aldehydes. Miscellaneous compounds are included in the most similar of the three categories. For each of these organics categories, LIRAQ uses about 10 reactions. The reactions and the reaction rates are chosen to represent the chemistry of an "average compound" in the respective chemical category.

The means of representing organics reactions in the Airshed Model is somewhat different from that used in LIRAQ. In particular, the categories used in the Airshed Model represent total numbers of bonds of specific bond types rather than total numbers of molecules of specific molecular types. In other words, the Airshed Model treats individual compounds not as molecular units but rather as carbon-bond units. Several different carbon-bond types are recognized: single bonds, double bonds, aromatic bonds, and carbonyl bonds. (These can be recognized as the identifying bond types for paraffins, olefins, aromatics and aldehydes.) The double bonds are further broken down into highly reactive and moderately reactive double bonds. The single bonds actually correspond to the number of carbon atoms which are only singly bonded. An aromatic bond is actually treated as an aromatic ring. Carbonyl bonds include not only those associated with aldehydes, but also those associated with ketones and esters. The single bonds are the least reactive while the highly reactive double bonds are, as their description implies, the most reactive; the others are of intermediate reactivity.

Another species which can be considered in the Airshed Model is CO. Carbon monoxide plays only a minor role in ozone photochemistry and most photochemical models consider it insignificant enough to ignore. Carbon monoxide has more significance as a relatively inert gas which may be used as a tracer. By comparing the CO concentrations estimated by the model to measurements of CO concentrations, it is possible to obtain a direct assessment of the accuracy of the treatments of emissions, advection, and dispersion without the complicating influence of chemistry. This can be quite useful for assessing model performance.

Another feature of the chemical mechanism is the option to consider temperature effects. Temperature has a significant effect on the rates at which many reactions occur, although it is unclear what effect it has on overall ozone production. Unfortunately, there is little known about the temperature dependence of the rates of many important photochemical reactions. Nevertheless, the Airshed Model does provide the option to utilize current knowledge about the temperature variation of the rate constants used in the chemical mechanism.

CHAPTER II. OVERVIEW OF THE MODELING PROCESS

A. ROLE OF MODELING IN AIR QUALITY PLANNING

The Clean Air Act requires the States to prepare State Implementation Plans (SIPs) for assuring that ambient air quality standards are met within a reasonable time frame by implementing various control measures on a progressive schedule. In the case of oxidants, the control measures thought necessary involve considerable expense to the community and may require significant changes in transportation and land use practices. While there are many elements involved in achieving public acceptance of and support for such measures, a fundamental element is the air quality planning and analysis which lead to their adoption. Decision-makers, legislators, and the concerned public must perceive the planning process as one in which due consideration is given to the technical aspects of the oxidant problem. Success hinges on credibility which in turn requires that recommendations for action be based on a firm technical foundation.

Modeling is a tool which enables air quality planners to demonstrate a cause and effect relationship between specific control measures and anticipated improvements in air quality. Photochemical grid models, such as the Airshed Model, simulate the physical and chemical processes which lead to observed oxidant levels in urban areas. Model results are verified against measured ozone data. The effects of a given emission reduction not only on peak ozone levels but also on its spatial and temporal distribution and on total population exposure can be determined. Using such a model, the air quality planning agency will have the information and tools at its disposal to prepare and defend with confidence its plan for achieving the ozone standard and improving public health.

Use of the Airshed Model is no small undertaking. The model requires substantial input data and lengthy computer runs to operate. A successful modeling study depends on the active participation of the air pollution control agency, the transportation planning agency, the regional planning agency, and all affected city and county governments.

The experience of the Association of Bay Area Governments (metropolitan San Francisco) in carrying out a detailed photochemical modeling study has been summarized in a report entitled "Application of Photochemical Models in the Development of State Implementation Plans, Volume I: The Use of Photochemical Models in Urban Oxidant Studies," (ABAG, 1979). Although a different model, LIRAQ was used, the planning considerations, data collection activities, and modeling aspects of the San Francisco application lend insight into the use of photochemical dispersion models more generally.

While the actual model application and much of the data collection may be done under contract, the study direction necessarily comes from the local agencies. The local agencies are also a primary source of information. The development of a suitable emission inventory for a base year along with projections of anticipated growth in future years requires the coordinated efforts of the regional planning agency, the pollution control agency, and the transportation planning agency. Because highway mobile sources are such a major contributor to the oxidant problem in urban areas, the use by the transportation agency of sophisticated transportation and emissions models is a critical element in the study. Collection of supplementary air quality and meteorological data requires the involvement of the pollution control agency. The selection of control measures to be evaluated and the selection of a final strategy requires the participation of all these bodies of government. Interaction of all affected groups will go far in assuring that the modeling study meets the needs of the community and results in an acceptable plan which, when implemented, achieves air quality goals.

B. SELECTION OF THE MODELING REGION

Before a photochemical modeling study can begin, it is first necessary to define the extent of the modeling region. In doing so, a number of criteria should be observed. In simplest terms however, the modeling region must be big enough to encompass the problem. Unfortunately, few urban areas have sufficient ozone monitoring data to determine the spatial extent of elevated ozone levels.

The modeling region should encompass the urban core and outlying suburban areas which together comprise the urban metropolitan area. It should also include significant satellite cities or towns and any major exurban industrial sources of oxidant precursors, e.g., hydrocarbon or nitrogen oxides. Allowance should be made to include areas where future growth is anticipated. In general, the modeling region should be large enough so as to include all major nearby upwind sources under meteorological conditions known to be conducive to elevated ozone levels.

Transport of oxidants and precursors into the metropolitan area from adjacent airsheds and formation of oxidants downwind of the metropolitan area are also important considerations when determining the extent of the modeling region. Transported ozone can significantly affect ozone levels in urban areas. As discussed in Chapter III, in order to quantify the importance of transport, it is necessary to locate supplementary ozone monitoring sites well upwind of the city. Similarly, ozone monitoring sites downwind of the urban area are necessary to determine ozone maxima resulting from ozone within the urban plume. In general, the modeling region should encompass both the upwind and downwind monitoring sites.

While the modeling region must be large enough to adequately study the urban oxidant problem, too large a region is undesirable. Emission inventory costs go up as the size of the modeling region increases. In addition, computer resource requirements for modeling are proportional to the total number of grid squares in the modeling region. A compromise must be reached between the size of the modeling region and the size of an individual grid square. Grid squares approximately 5 kilometers on a side are needed. In general, the larger the grid size, the more localized effects are smoothed over and the less useful information is provided by the model. By orienting the modeling region in an upwind-downwind direction, it may be possible to reduce the size of the region while retaining the desired grid size. Figure II-I shows the modeling region being used for an Airshed Model application in metropolitan Philadelphia.

C. COLLECTION OF AEROMETRIC AND EMISSIONS DATA

Use of the Airshed Model in an urban area requires a large aerometric and emissions data base. Existing data bases are almost universally inadequate in important respects, thus necessitating the collection supplementary emissions, air quality, and meteorological data. The required spatial resolution of a modeling data base is on the order of 5 kilometer grid squares while the required temporal resolution is on the order of 1 hour. Data collection programs must be designed with these modeling

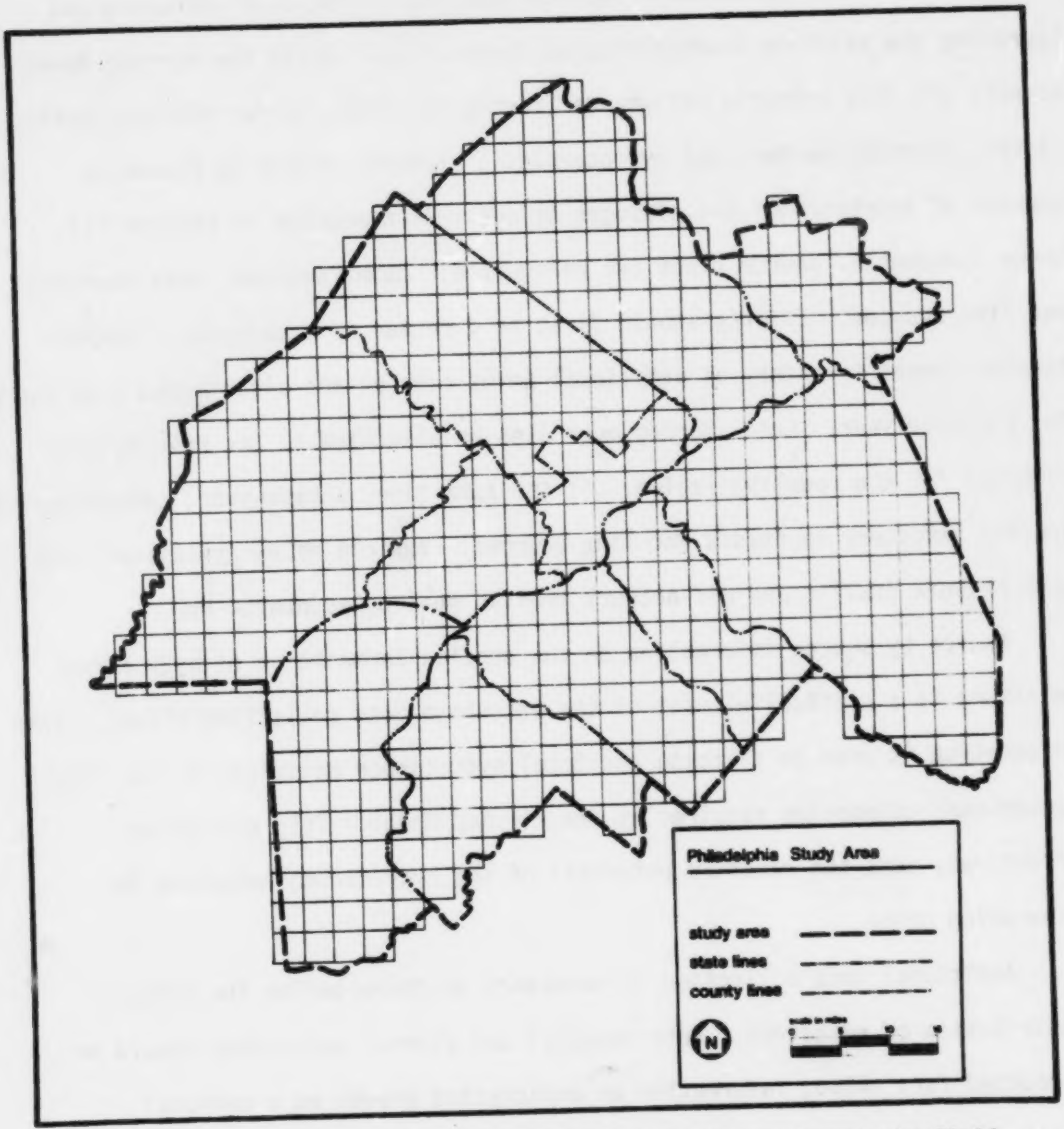

Philadelphia Study Area
study area
state lines
county lines
N
scale in miles

Figure II-1. Example of a Modeling Region and Grid Specification for an Airshed Model Application (adapted from Engineering-Science, 1979b).

needs in mind. The Airshed Model, as discussed in Chapter IV, offers extensive data preparation programs which help make the best use of the data collected.

Collection of source and emissions data should focus on upgrading and improving the existing source/emission inventories. While the Airshed Model accepts all five criteria pollutants (carbon monoxide, sulfur dioxide, particulates, nitrogen oxides, and hydrocarbons), emphasis should be placed on sources of hydrocarbons and nitrogen oxides. As discussed in Chapter III, three fundamental source types are recognized: point sources, area sources, and line sources. Efforts should first be directed at developing a comprehensive annual inventory of individual point sources and distributed area sources for the base year. Area sources must also be allocated to the grid network selected for the modeling region. At the same time, a base-year, comprehensive traffic inventory is needed for line sources. Vehicle miles associated with both network traffic and off-network traffic must be accounted for.

Source by source information on the species composition of hydrocarbon emissions is a critical element of the emissions data collection effort. This information is used to allocate the total hydrocarbon emissions to the five carbon-bond categories required by the Airshed Model. This allocation effectively sets the reactive potential of the hydrocarbon emissions in generating ozone.

Additional data collection is necessary to characterize the temporal distribution of emissions. Both seasonal and diurnal variations should be accounted for. Also, information on anticipated growth on a regional scale is needed to project the base year emissions to future years. The final goal is an hourly emissions inventory of all sources, for the base year and the projection years that is representative of a weekday during the "oxidant season."

Collection of aerometric (meteorological and air quality) data should focus on supplementing the existing monitoring network. This is generally done in the form of a comprehensive "summer study." Such a study should last about three months during the oxidant season so that a variety of high-ozone episodes are represented. Air quality and meteorological data are gathered on a ground-based network consisting of both existing and supplementary monitoring sites. Continuous ozone, nitrogen dioxide/nitric oxide, and nonmethane hydrocarbon monitors are used to characterize ground-level air quality. Meteorological instruments for measuring wind speed and direction, temperature, and solar insolation are variously collocated with the air quality monitors. Rawinsonde and pibal releases are used for characterizing upper-level winds, mixing height, and stability. In addition, aircraft overflights are desirable in some metropolitan areas in order to characterize air quality aloft. Finally, grab samples are collected and analyzed for individual hydrocarbon species in order to further characterize the ambient reactive mix.

As discussed in Chapter III, the air quality data is needed both to specify the initial and boundary conditions for model application and to evaluate and verify the model's performance at estimating ozone levels in the base year. The meteorological data is necessary to prepare mixing heights and a three-dimensional wind field which, together with emissions, are the major driving forces which control the model predictions.

D. MODEL VERIFICATION AND CONTROL STRATEGY ANALYSIS

One of the key features of using a photochemical grid model such as the Airshed Model is that model results are verifiable: model estimates of ambient ozone concentrations can be compared directly with observed concentrations. Various statistical and graphical performance measures may then be employed to assess whether the model is performing satisfactorily.

Model verification is conducted for the base year. In other words, the base year emission inventory together with the aerometric data collected during the base year summer study are used to prepare the model input data. A total of eleven data files must be prepared prior to running the simulation program; several other nondata files are also required. The Airshed Model includes a variety of data preparation programs. However, not all the methods and options offered may be sufficient or appropriate for a particular application, necessitating modifications of the existing programs or writing of new ones.

Several days during the summer study period should be selected for model verification. Such factors as ozone levels and data completeness should be considered, among others. Simulation of more than a single day allows one to evaluate how the model performs for a range of conditions under which high ozone concentrations occur. Moreover, satisfactory model performance may not be achievable on a particular day causing one to turn to other days. The emissions data base is not normally developed for a specific calendar day, but rather for a representative weekday. However, the meteorological and air quality data must be prepared separately for each calendar day for which a simulation is to be run.

Model verification requires a high level of skill and judgment on the part of the modeler in addition to an intimate familiarity with the data base.

Verification is an iterative process whereby model executions are followed by an evaluation of the model's performance, a diagnosis of any problems, and a reanalysis of the model input data. Modifications are made, the model is rerun, and the process is continued until satisfactory performance is achieved on one or more days.

Once the model and data base have been verified, the Airshed Model is ready to be applied to the analysis of control strategy options. This step is the culmination of all previous steps where the benefits of the photochemical modeling study are realized. The question of what control measures should be imposed on which sources with what level of stringency may be answered using the Airshed Model as an analysis tool.

Control strategies are evaluated for a critical test day when the mesoscale meteorology, pollutant transport, and pollutant carryover (from previous days) result in high ozone levels. Control strategies may be formulated using a sensitivity approach to determine an overall regional emission reduction or by a more rigorous approach in which candidate strategies are simulated. Control strategy evaluation should be conducted for several test days of different meteorological and air quality data. The effectiveness of a particular control strategy may vary depending on the aerometric conditions on a particular test day. The ultimate goal is a control strategy consisting of specific control measures for specific sources which, by means of model simulation, is shown to attain the ozone standard on each of the high-ozone test days.

CHAPTER III. DATA NEEDS

A. SOURCE AND EMISSION INVENTORIES

The Airshed Model and other photochemical grid models attempt to simulate the production, decay, and transformation of multiple pollutants in a reactive atmosphere. In order to portray this reactive mix over time, it is necessary to estimate the total emissions of photochemically reactive pollutants and their spatial and temporal distribution. The principal reactive pollutants affecting ozone formation are hydrocarbons and nitrogen oxides. The Airshed Model requires an hourly breakdown of the total ground-based emissions and elevated emissions of these pollutants for each grid square. In addition, emissions of carbon monoxide are also useful during the modeling study.

1. Requirements for Source and Emissions Data

As indicated in Table III-1, emission sources are generally broken down into three categories: line sources, area sources, and point sources. Line sources consist of motor vehicle emissions from streets and highways. In terms of transportation planning, line sources encompass both link VMT (vehicle miles traveled) associated with vehicle trips on the transportation network and intrazonal VMT associated with trips off the network. Line sources are the single most important source of precursor emissions in urban areas. Area sources consist of numerous small stationary source emissions and off-highway mobile source emissions. Point sources consist of stationary sources of varying size which are individually identified in detail. While the Airshed Model itself requires only emission rates, collection and storage of the source

Table III-1

Source and Emissions Data Needs

Category	Data
Line Sources	Network Links hourly link emissions;* endpoint locations; vehicle mix and model year mix; diurnal pattern of VMT, average speed, and % hot and cold starts; other auxiliary data; VOC and NO_x species data.
	Intrazonals (off-network) hourly zone emissions;* grid allocation factors; other data as above.
Area Sources	annual county-level emissions* and activity levels; grid allocation factors; temporal apportioning factors, VOC and NO_x species data.
Point Sources	plant identification; point identification; annual point emissions;* locations; stack parameters; control efficiencies; process identification and operating rates; temporal apportioning factors; VOC and NO_x species data.

*Emissions of HC, NO_x, and CO.

data indicated in Table III-1 is needed to perform the computations necessary to project emissions to future years, both to examine the effect of growth and of additional control measures, and to prepare the data for model input.

The necessary procedures for developing the kinds of data shown in Table III-1 have been discussed elsewhere. "Procedures for the Preparation of Emission Inventories for Volatile Organic Compounds, Volume I" (EPA, 1977b) describes the methods used for compiling annual inventories of VOC emissions from point and area sources. However, the methods for inventorying area sources are intended for relatively large geographic areas, such as counties. A companion document, Volume II, is entitled "Emission Inventory Requirements for Photochemical Air Quality Simulation Models," (Pacific Environmental Services, 1979). It describes requirements and methodologies for developing an inventory of point, area, and line (i.e., highway mobile) sources for use in photochemical grid models, such as the Airshed Model. For point and area sources, the spatial and temporal resolution in Volume II builds on the basic annual inventory of Volume I. However, for highway mobile sources, a completely different procedure is recommended which is based on the use of transportation models and network emission models. Volume II also provides a general description of VOC species data. However, the use of such data for an Airshed Model application is described here. The following provides an overview of the inventory process and highlights the salient features an inventory should possess if it is to be used for an Airshed Model application.

In general, a metropolitan area planning to undertake a photochemical modeling study should already have most of the basic source/emissions inventory information in some form. However, it is usually necessary to update the point and area source inventories, assemble the various data elements for the line source inventory, develop grid allocation factors for area sources, and conduct original surveys of point or area source categories not currently accounted for. A good annual inventory is the necessary starting point for area and point sources while a good transportation inventory is necessary for line sources.

Updating of the point and area source inventories should focus on sources of hydrocarbons and nitrogen oxides. Table III-2 lists the principal sources of these pollutants in urban areas. While the point source inventory identifies individual, discrete processes, the area source category breakdown used depends upon the relative similarity of different sources. Different allocation parameters, temporal patterns, organic species compositions, or emission factors may dictate subdivision of the categories listed in Table III-2. For example, the different solvents used for drycleaning have different chemical compositions and different reactivities. When allocating the solvent emissions to the five carbon-bond categories, a stoddard solvent is treated differently than perchoroethylene. In addition, consideration should be given to the control measures to be evaluated. For example, if stage I and stage II service station controls are to be analyzed separately, then it may be desirable to subdivide service station emissions into those associated with loading underground tanks and those associated with automobile tank filling.

Once the point, area, and line source inventories are assembled, the emissions must be apportioned to hourly periods. The hourly emissions should be representative of a typical weekday during the oxidant season (usually June through September). Original surveys of hourly process rates for the major point sources of hydrocarbons and nitrogen oxides are desirable. For smaller point sources, plant operating schedules are sufficient to derive typical hourly emissions, while for area sources temporal patterns for each

Table III-2

Sources of Hydrocarbon and Nitrogen Oxide Emissions

PETROLEUM REFINERIES

- Process Drains and Wastewater Separators
- Vacuum Producing Systems
- Process Unit Turnaround
- Boilers and Process Heaters
- Catalytic Cracking
- Chemical Treating
- Coking
- Blending
- Air Blowing
- Fugitive Sources

STORAGE, TRANSPORTATION, AND MARKETING OF PETROLEUM PRODUCTS

- Oil and Gas Production Fields
- Natural Gas and Natural Gasoline Processing Plants
- Pipelines
- Petroleum Product Storage[a]
- Ship and Barge Transfer of Gasoline and Crude Oil
- Bulk Gasoline Terminals[b]
- Gasoline Bulk Plants[c]
- Service Station Loading[d]
- Service Station Unloading[e]

ORGANIC CHEMICAL MANUFACTURE[f]

- Process Streams
- Storage and Handling
- Waste Handling
- Fugitive Sources

INDUSTRIAL PROCESSES

- Paint, Varnish, and Ink Manufacture
- Food Processing
- Pharmaceutical Manufacture
- Rubber Products Manufacture
- Plastic Products Manufacture
- Textile Polymers Manufacture
- Coke Production
- Mineral Products Manufacture
- Nitrate Fertilizer Manufacture
- Nitric Acid Manufacture
- Explosives Manufacture

Table III-2 (continued)

INDUSTRIAL SURFACE COATING

- Large Appliances
- Magnet Wire
- Automobiles
- Cans
- Metal Coils
- Paper
- Fabrics
- Metal Furniture
- Wood Furniture
- Flat Wood Products
- Other Metal Products

NONINDUSTRIAL SURFACE COATING

- Architectural Coatings
- Auto Refinishing

OTHER SOLVENT USE

- Degreasing (toluene, trichloroethylene, and other)
- Dry Cleaning (stoddard, perchloroethylene, and other)
- Graphic Arts
- Adhesives
- Cutback Asphalt Paving
- Miscellaneous Commercial/Consumer Solvent
- Pesticides

STATIONARY SOURCE COMBUSTION

- External Fuel Combustion
  - Electric Generation
  - Industrial Boilers
  - Commercial and Institutional Boilers
  - Residential Heating
- Internal Fuel Combustion
  - Turbine
  - Reciprocating Engine
- Solid Waste Combustion
  - On-Site Incineration
  - Open Burning

HIGHWAY MOBILE SOURCES

- Link VMT
  - Light Duty Autos
  - Light Duty Trucks
  - Heavy Duty Gasoline Trucks
  - Heavy Duty Diesel Trucks
  - Motorcycles
- Intrazonal VMT
  - Same as above

Table III-2 (continued)

OFF-HIGHWAY MOBILE SOURCES

- Railroads
- Aircraft
- Vessels
- Construction Equipment
- Agricultural Equipment
- Other Vehicles

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[a] Petroleum Product Storage--includes all storage facilities except those at service stations and gasoline bulk plants.

[b] Bulk Terminals--emissions from loading tank trucks and rail cars.

[c] Bulk Plants--emissions from storage and transfer.

[d] Service Station Loading--filling of underground storage tanks.

[e] Service Station Unloading--automobile tank filling.

[f] Organic Chemical Manufacture--only generic classes of processes associated with the manufacture of various organic chemicals are listed.

type of activity are needed. For line sources, hour-by-hour traffic counts representative of various roadway functional classes (freeway versus arterial, etc.) and locale (central business district versus suburban residential, etc.) are needed to characterize the diurnal distribution of VMT.

Except when stack tests or materials balance calculations show otherwise, standard AP-42 (EPA, 1977a) emission factors can usually be used for estimating emissions for point and area sources. Occasionally other references may be required for certain source categories. For line sources, the MOBILE1* computer program (EPA, 1978a&b) should be used for generating mobile source emission factors. Most point and area source emission factors are assumed constant with time. However, emission factors for highway mobile sources vary diurnally as vehicle operating conditions change over time. Both average vehicle speed (as correlated with traffic loading) and percent hot and cold starts show distinct variations from hour to hour and have a marked effect on motor vehicle emissions. Therefore, hourly variations in emissions from links and intrazonals are a result of hourly changes in both VMT and emission factors.

The Airshed Model requires that hydrocarbon emissions be apportioned to the five carbon-bond categories discussed in Chapter I in order to properly treat the varying reactivity of different organic species. It is therefore necessary to obtain organic species (VOC) data for each source or source type. Publications are available which give typical organic profiles for a wide variety of point and area source types in terms of the weight or volume percent of the individual organic compounds present [Bucon, Macko, and Taback (1978); Griscom (1978); Trijonis and Arledge (1976)]. Highway mobile source exhaust profiles depend on whether the vehicle is catalyst equipped and therefore on the type of fuel burned. Exhaust profiles are obtained from the same publications as are profiles for the evaporative portion of gasoline vehicle emissions and diesel vehicle exhaust emissions.

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*A revision of MOBILE1 is expected in July, 1980.

Despite the utility of these publications, probably the best data, at least for point sources, would be obtained from responses to questionnaires sent out to individual sources. Much of the published data is for the Los Angeles area and may not be applicable to other parts of the United States. For example, surface coating operations exhibit large variations depending on the solvent or coating used. In addition, gasoline composition is significantly different in California than it is elsewhere. Profiles for gasoline storage and handling, as well as for highway vehicles, should reflect the local average gasoline composition. In the case of highway vehicles, published profiles may be adjusted depending on the composition of the gasoline (Engineering-Science, 1979). For sources where no data are available at all, an alternative may be to use the urban ambient mix of organic species (as discussed in Section B. Air Quality Data of this chapter) as a surrogate profile.

A note of caution regarding hydrocarbon emissions is in order. Most hydrocarbon emission factors reported in the standard reference AP-42 do not account for aldehyde emissions. A few source types have aldehyde emission factors reported separately in AP-42, but most do not. Therefore, it is generally necessary to adjust the emissions of sources which emit aldehydes, primarily stationary and mobile source combustion, to obtain total hydrocarbon emissions. This may be done as follows:

$$\text{Adjusted HC Emissions} = \text{HC Emissions} \left(\frac{100}{100\text{-weight \% aldehyde}^{*}} \right)$$

*as formaldehyde (HCHO)

This adjustment is made prior to apportioning the emissions to the five carbon bond categories, which is discussed below.

The data needed to develop a profile in terms of the five carbon bond categories used by the Airshed Model is (1) the weight percent and (2) the molecular weight of each species present. If the data are reported in terms of volume percents, it may be readily converted to weight percents. The data are then used to compute first, the number of moles of each species present, and second, the number of moles of each bond type associated with each species. Once the moles of bond types are computed for all species, they are summed to obtain the total number of moles of each bond type. The data manipulations involved are described further in the Appendix, Technical Description of the Airshed Model.

While the technique just described is recommended when detailed species by species data is available, it may be found that some summarization of the data by organic class has been undertaken prior to reporting the data. If so, the calculations necessary to obtain the five carbon bond categories will depend on the classes actually reported. For example, if the data have been summarized in terms of paraffins, olefins, aldehydes, ketones, alcohols, acetates and aromatics, the equations in Table III-3 could be used to approximate the carbon-bond categories.

The Airshed Model also requires that nitrogen oxides be apportioned to the two species, NO and NO_2. Little data are available regarding the relative proportion of nitric oxide and nitrogen dioxide in emissions from combustion sources. However, some data for stationary sources has been published (Milligan, et al., 1979) and data used in preparing a photochemical inventory for Tulsa have been reported (Engineering-Science, 1979).

While the above data items are needed for each source to derive a temporally resolved inventory of the various pollutants required by the Airshed Model, further data is needed to provide the appropriate level of

Table III-3. Possible Equations for Estimating Airshed Model Carbon Bond Categories

Carbon Bond Category		Equation
(1) OLE	=	$\frac{\text{mass olefins C3+}}{\text{MW olefins C3+}}$
(2) ARO	=	$\frac{\text{mass aromatics}}{\text{MW aromatics}}$
(3) CARB	=	$\frac{\text{mass aldehydes}}{\text{MW aldehydes}} + \frac{\text{mass ketones}}{\text{MW ketones}} + \frac{\text{mass acetates}}{\text{MW acetates}}$
(4) PAR	=	$\frac{\text{mass paraffins}}{14} \left(\frac{\text{MW paraffins} - 2}{\text{MW paraffins}}\right)$
		$+ \frac{\text{mass olefins C3+}}{14} \left(\frac{\text{MW olefins C3+} - 28}{\text{MW olefins C3+}}\right)$
		$+ \frac{\text{mass aromatics}}{14} \left(\frac{\text{MW aromatics} - 78}{\text{MW aromatics}}\right)$
		$+ \frac{\text{mass aldehydes}}{14} \left(\frac{\text{MW aldehydes} - 30}{\text{MW aldehydes}}\right)$
		$+ \frac{\text{mass ketones}}{14} \left(\frac{\text{MW ketones} - 30}{\text{MW ketones}}\right)$
		$+ \frac{\text{mass acetates}}{14} \left(\frac{\text{MW acetates} - 46}{\text{MW acetates}}\right)$
		$+ \frac{\text{mass alcohols}}{14} \left(\frac{\text{MW alcohols} - 18}{\text{MW alcohols}}\right)$
(5) ETH	=	$\frac{\text{Mass olefins C2}}{28}$

Notes: Units of Carbon Bond categories are gram moles.

Units of mass are grams.

MW is the average molecular weight of the class of compounds indicated.

spatial resolution. As discussed previously, the Airshed Model requires, in general, a gridded inventory. However, the model will accept individual point sources. It is not necessary or desirable to treat all point sources individually for modeling purposes. Rather, point sources should be separated into "major" sources and "minor" sources. Only the major point sources are left as individual sources. The minor point sources are assigned to grids and their emissions are aggregated. Two criteria should be observed when selecting the major point sources. First, the emissions should be released into an elevated layer, at least 50 meters or more above the surface. Second, the quantity of hydrocarbon or nitrogen oxide emissions should represent a significant fraction of the regional total emissions, on the order of one half of one percent. In this regard, it is not so much the emissions from an individual source, but rather the total amount of elevated emissions within a column of grid cells that is important.

As with minor point sources, line sources and area sources must be assigned to the grid squares. Link emissions are readily assigned on the basis of their endpoint coordinates. Where a link falls in two or more grids, the emissions may be apportioned on the basis of the fraction of the length of the link in each grid. Intrazonal line source emissions may be apportioned according to the fraction of the area of the zone in each grid.

A variety of surrogate indicators are used to apportion county area source emissions to the grid squares. For example, population might be used for apportioning domestic solvent emissions, commercial land use for gasoline handling, and basic employment (as compared with service employment) for degreasing emissions. In this example, population, commercial land use, and basic employment are termed allocation parameters. The fraction of the county total of each parameter associated with each grid square is an allocation factor. Obviously, this approach presumes that data for the allocation parameters are available at a "sub-county" level. Census data along with transportation, land use, and economic studies oftentimes provide such data for individual analysis zones of sufficient spatial resolution for use in photochemical modeling. Of course, if the specific locations of area sources are known, the use of surrogates is unnecessary. This may be the case for diesel locomotives, where track mileage and switchyard locations are known, aircraft emissions where airport locations and relative levels of activity are known, and gasoline handling where a survey of service stations has been undertaken.

2. Emission Projections

A good base year emission inventory as described above is necessary in order to verify the model's performance (Chapter V, Evaluation of Model Performance). However, its primary importance is actually as a starting point from which to project future emissions. Emission projections serve as the basis for systematic planning to attain air quality goals. Two types of projected inventories are recognized: (1) baseline projection inventories, and (2) strategy projection inventories.

Baseline projections include the effect of growth and control regulations now in effect. Their purpose is to estimate where an urban area will be in terms of emissions and air quality at some future date if no additional controls are adopted. The need for additional controls can then be assessed. While no one has a crystal ball, it is possible with suitable techniques and assumptions to estimate future emissions in a meaningful way.

Baseline projections are usually done separately for point, area, and line sources. Point and area source projections are generally the responsibility of the air pollution control agency while line source projections should be done by the transportation planning agency. Coordination is necessary to assure that projections are done on a consistent basis.

For consistency, all growth projections, whether point, area, or line, should be derived from the same basic social and economic indicators. Such indicators include population, employment, housing and land use. Regional growth models, such as IPEF (Interactive Population/Employment Forecasting Model) are used to forecast regional population and employment. These forecasts are then used together with information on land use, transportation, and planning policy to forecast land use, population, employment, and housing in individual transportation zones with a model such as PLUM (Projective Land Use Model). These models are available from the Federal Highway Administration and are often used by transportation planners as basic inputs to the transportation modeling process. For projections of stationary source emissions such forecasts are invaluable, not only in and of themselves, but also as regional control totals. Ideally, projections of both mobile and stationary source emissions, at a regional level, should be firmly tied to these fundamental indicators of growth.

Transportation models use these social and economic indicators to estimate trip generation and distribution in future years. Once these trips are assigned to a planned future highway network, the resulting traffic loadings can be used to calculate emissions. (If the transportation model has not been run for precisely the same year(s) which interest air quality planners, it may be possible to interpolate from the results for years which have been run. If this is attempted however, it should be done by the transportation planning agency to assure its validity.) Revised vehicle speeds appropriate for loadings on the future network should be used in selecting emission factors, as should revised percent cold starts and hot starts in areas where land use is projected to shift substantially.

Point and area source projections are usually done on a source category by source category basis using the best information available. Changes in gasoline marketing might be estimated on the basis of total projected VMT (from the transportation model) and average projected fuel economy. Changes in petroleum refining might be based on a judgmental application of national trends, on projected changes in local basic employment, or on the basis of a local survey of the industry. Unless information to the contrary is available, it is generally necessary to assume that all emission points in a large industrial facility "grow" by the same factor. Only for a few sources, such as power plants, is sufficient information generally available on planned new sources or facility expansions to make possible the actual addition of new emission points to the inventory.

Normally overall growth and the effect of control measures on area source emissions are projected at the county level (or at a redefined "political jurisdiction" level) while changes in area source spatial patterns are handled through the use of allocation factors developed specifically for a certain projection year. Most area source categories are projected using such surrogates as population, employment and land use forecasts and are then allocated to grids using the same surrogates. It is therefore possible to develop corresponding allocation factors for a specific projection year.

Strategy projections, as discussed in Chapter VI, Model Application for Air Quality Planning, are used to evaluate the effectiveness of additional proposed control measures and to test the final strategy selected for attainment of the ozone standard. Typical control measures that may be considered include reasonably available control technology (RACT), lowest achievable emission rate (LAER), and best available retrofit technology (BART) for point and area sources. Inspection and maintenance (I/M) and transportation control measures (TCMs) may be considered for line sources.

The level of control represented by RACT, for example, when applied to a given source category, may be expressed as a control factor which is then used to reduce the projected (baseline) emissions to arrive at the controlled (strategy) emissions. When controls already exist, it is probably best to start from the uncontrolled level and then apply the appropriate reduction. A complication arises when, for example, it is desired to apply a level of control corresponding to LAER to new sources while applying a level corresponding to RACT to existing sources of the same category. If growth is anticipated, yet specific information on new units does not exist or is unavailable, it may be necessary to make some simplifying assumptions about how much of the growth is "new" and how much is due to an increase within existing capacity and therefore "old." When making longer-term projections, say to 1995, replacement of existing capacity may be another complicating factor.

While the simplifications and assumptions required are not insignificant, the degree of detail with which projections are performed should be commensurate with the accuracy of the growth indicators from which they are derived. Moreover, what is important from a modeling viewpoint is the total regional change in emissions and its spatial and temporal distribution.

3. Emissions Data Handling

The above discussion has outlined the wide variety of data required for the base year and projection year inventories. This data is used to generate an hourly inventory of eight pollutants (NO, NO_2, five carbon-bond categories, and CO) for each grid square in the modeling region along with an inventory of hourly emissions for each major point source.

Assume for the moment that the modeling region contains 400 grid squares and 50 major point sources. For a fourteen hour simulation the Airshed Model requires emissions for eight pollutants for each hour. The number of emission values input to the model is therefore 400 grids x 8 pollutants x 14 hours/day plus 50 points x 8 pollutants x 14 hours/day or a total of 50,400 values. Each of these 50,400 values is generated from a series of calculations. These 50,400 values would then have to be regenerated for each baseline projection and strategy projection to be simulated. Obviously, some form of computer assisted procedure is necessary to perform the literally millions of calculations and manipulations necessary.

A schematic representation of a computerized procedure for performing the necessary calculations and converting the results to model format is shown in Figure III-1. The procedure requires as input an EIS/P&R file of point and area source emissions. Due to its design, the EIS/P&R system (EPA, 1975) is quite flexible and well suited as the starting point from which an Airshed inventory of point and area source emissions may be developed. Line sources should be handled separately however; this is discussed later.

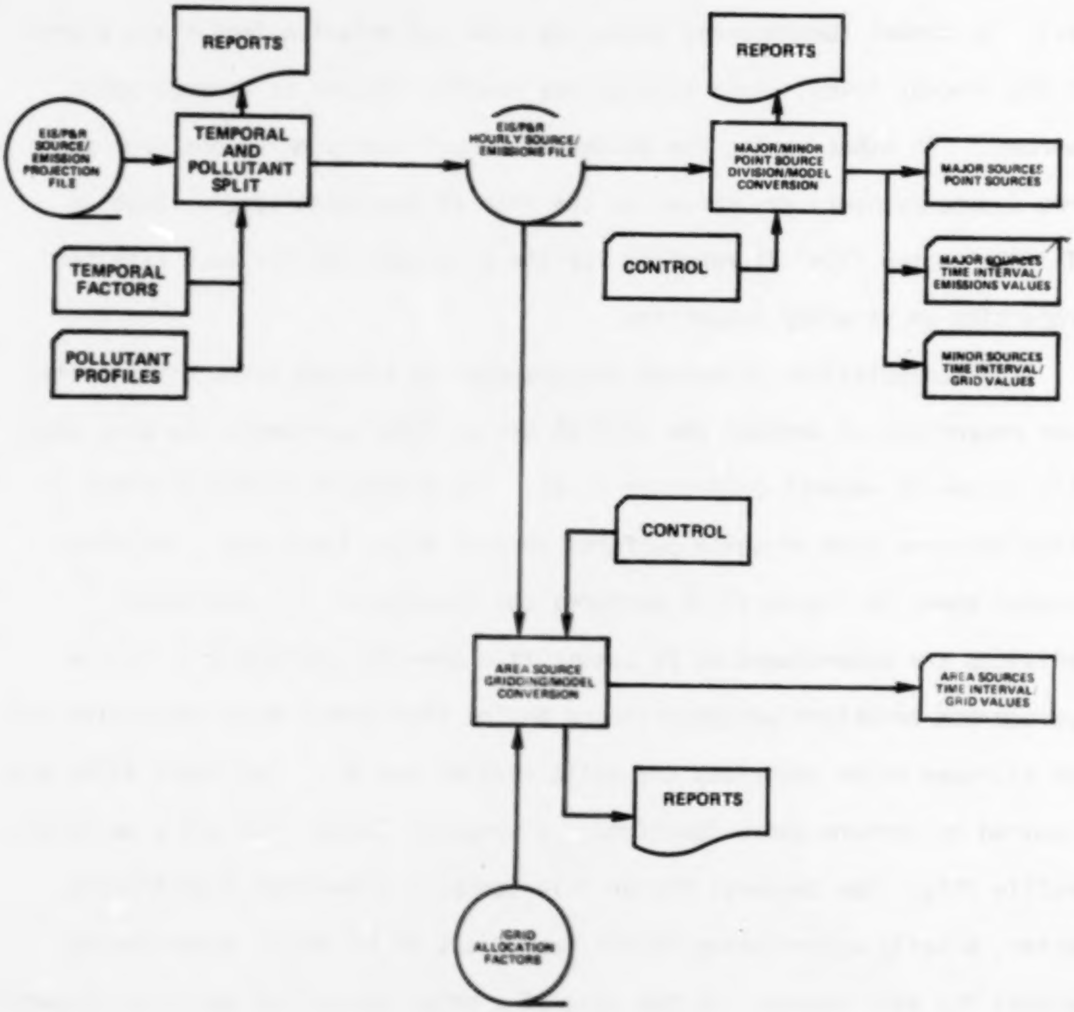
REPORTS
EIS/P&R SOURCE/ EMISSION PROJECTION FILE
TEMPORAL AND POLLUTANT SPLIT
TEMPORAL FACTORS
POLLUTANT PROFILES
EIS/P&R HOURLY SOURCE/ EMISSIONS FILE
REPORTS
MAJOR/MINOR POINT SOURCE DIVISION/MODEL CONVERSION
CONTROL
MAJOR SOURCES POINT SOURCES
MAJOR SOURCES TIME INTERVAL/ EMISSIONS VALUES
MINOR SOURCES TIME INTERVAL/ GRID VALUES
CONTROL
AREA SOURCE GRIDDING/MODEL CONVERSION
AREA SOURCES TIME INTERVAL/ GRID VALUES
REPORTS
/GRID ALLOCATION FACTORS

Figure III-1. A POINT AND AREA SOURCE DATA HANDLING PROCEDURE.

The EIS/P&R file has a hierarchical structure. Each facility or "plant" may contain several "points" defined as stacks or boilers. Each point may contain several processes or "SCCs." The SCC or Source Classification Code (EPA, 1976) identifies the kind of process venting to a stack or, in the case of boilers, the type of boiler and the fuel burned. For point sources, stack data, operating schedule information, control efficiency, and annual estimated emissions are stored at the point level while the annual fuel/process operating rate and emission factor are stored at the process level. Area sources are readily treated as "pseudo-point sources." In other words, the estimated annual county emissions from each area source category are stored on the file at the point level. Such an EIS/P&R "master file" is required for the base year and for each baseline projection or strategy projection.

The manipulations necessary to generate the Airshed inventory are the same regardless of whether the EIS/P&R master file represents the base year file or one of several projection files. The procedure itself consists of three programs each of which performs several major functions. The first program shown in Figure III-1 performs two functions: (1) the annual emissions are apportioned to 24 consecutive one-hour periods and (2) the hydrocarbon emissions are apportioned to the five carbon-bond categories and the nitrogen oxide emissions are split into NO and NO_2. Two input files are required to perform these functions: a temporal factor file and a pollutant profile file. The temporal factor file contains a seasonal apportioning factor, a daily apportioning factor, and a set of 24 hourly apportioning factors for each source. In the case of a point source for which no temporal factors are input, the operating schedule information on the EIS/P&R master file is used instead. The pollutant profiles may be input source by source, or by source category. The profiles contain the weight percent of NO and NO_2 and weight percents for each of the five carbon-bond categories. (The development of these percents is described in the Appendix, Technical Description of the Airshed Model.) The pollutant profile file also contains the weight percent of aldehydes. This is used to perform the aldehyde correction discussed in Section 1. Requirements for Source and Emissions Data.

The second program in Figure III-1 divides up the point sources into major sources and minor sources. The user specifies a ton per year cut-off for both NO_x and HC and a plume height cut-off. Point sources exceeding these cut-offs then become major sources. The program then takes the major sources and creates two files in Airshed Model format, one containing the stack data for each source and the other containing the corresponding hour-by-hour emissions. The minor sources are assigned to the modeling region grid, the grid being defined by the user, and a file is created in model format containing hour-by-hour emissions for each grid square.

The third program takes the county area source emissions and disaggregates it into gridded emissions. The user inputs a file containing a set of allocation factors for each allocation parameter. These factors represent the fraction of each parameter, e.g., population, in each grid square. The user also specifies which allocation parameter is to be used for allocating which area source category, e.g., population, for domestic solvent use. The program then creates a file in model format containing hour-by-hour area source emissions for each grid square.

While a data handling procedure of the type just described is suitable for point and area source emissions, a different procedure is required for line sources. Figure III-2 shows a conceptual flow diagram for such a procedure. The procedure consists of several parts. First, as shown across the top of the figure, link emissions are calculated. Intrazonal emissions are also calculated and then combined with the link emissions when the emissions are allocated to grid squares.

The computation of link emissions begins with a file of transportation network data, a Federal Highway Administration (FHWA) "historical record" file for example. Diurnal traffic distributions are then used to compute hourly link traffic volumes. These volumes are used along with link capacity to estimate hour-by-hour link speeds. The volumes are also used to compute hour-by-hour VMT. This data, along with the other transportation data, is stored on the "Hourly Link File." Next, the MOBILE1 program is used to compute hour-by-hour emission factors for each link. Speeds are obtained from the "Hourly Link File" while percent cold starts and hot starts, ambient temperature, and a variety of other input parameters required by MOBILE1 are input separately. The percent cold starts and hot starts are input for each traffic zone, land use classification, or locale type. A preprocessor program selects the necessary MOBILE1 parameters for each link. The result is an hour-by-hour, link-by-link emission factor file. By multiplying these emission factors times the hour-by-hour VMTs from the "Hourly Link File," the hourly link emissions are computed. A similar procedure is used to compute intrazonal emissions.

Because evaporative emissions have a distinctly different organic composition than do exhaust emissions, evaporative and exhaust emissions

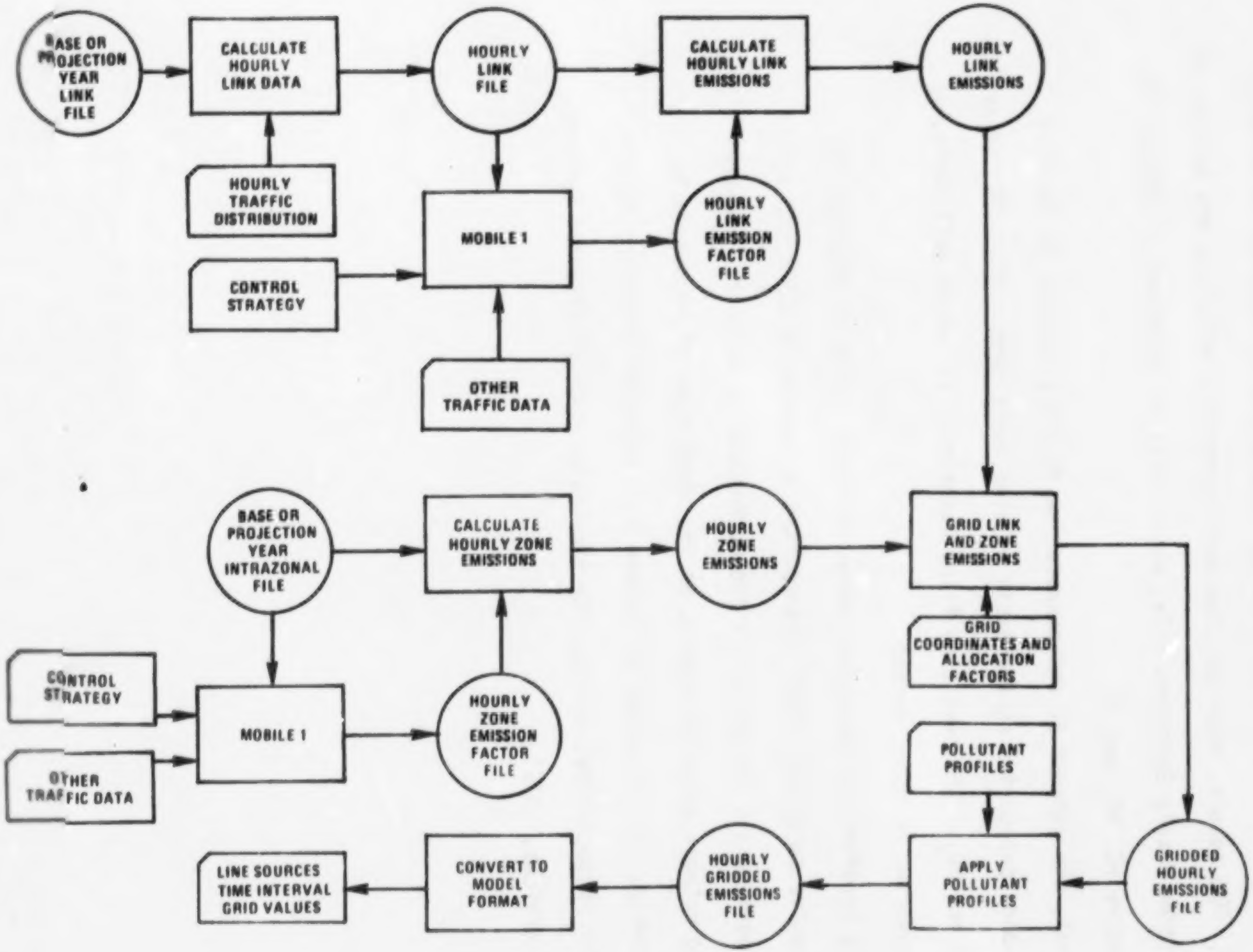
BASE OR PROJECTION YEAR LINK FILE
CALCULATE HOURLY LINK DATA
HOURLY LINK FILE
CALCULATE HOURLY LINK EMISSIONS
HOURLY LINK EMISSIONS
HOURLY TRAFFIC DISTRIBUTION
MOBILE 1
HOURLY LINK EMISSION FACTOR FILE
CONTROL STRATEGY
OTHER TRAFFIC DATA
BASE OR PROJECTION YEAR INTRAZONAL FILE
CALCULATE HOURLY ZONE EMISSIONS
HOURLY ZONE EMISSIONS
GRID LINK AND ZONE EMISSIONS
GRID COORDINATES AND ALLOCATION FACTORS
CONTROL STRATEGY
MOBILE 1
HOURLY ZONE EMISSION FACTOR FILE
OTHER TRAFFIC DATA
POLLUTANT PROFILES
LINE SOURCES TIME INTERVAL GRID VALUES
CONVERT TO MODEL FORMAT
HOURLY GRIDDED EMISSIONS FILE
APPLY POLLUTANT PROFILES
GRIDDED HOURLY EMISSIONS FILE

Figure III-2. A Line Source Data Handling Procedure.

are accounted for separately throughout the procedure. Therefore, the hourly emission factor files contain both an exhaust and an evaporative emission factor. The result, once the link and intrazontal emissions are merged, is the Gridded Hourly Emissions File, which contains emissions of exhaust HC, evaporative HC, NO_x and CO.

Next, the exhaust HC and evaporative HC are allocated to the five carbon-bond categories on the basis of user input data. Also, NO_x is split into NO and NO_2. The resulting file, containing all eight pollutants, is then converted to model format.

The hypothetical procedure shown in Figure III-2 is intended for illustrative purposes. Each transportation agency is likely to select and/or develop its own procedure and corresponding software. Several existing network emission models, as the above type of procedure is often termed, are discussed in "Volume II. Emission Inventory Requirements for Photochemical Air Quality Simulation Models" (Pacific Environmental Services, 1979).

B. AIR QUALITY DATA

In order to simulate the time history of pollutant concentrations, it is necessary to know or estimate the mass of pollutants entering from outside the modeling region. These "boundary conditions," expressed as concentrations, represent the transport of pollution, both ozone and precursors, into an urban area from upwind sources. In addition, "initial conditions" must be specified as discussed in Chapter I, Principles of the Airshed Model. In other words, the mass of pollutants existing within each grid cell of the modeling region at the start of the simulation must be known or estimated, again in terms of concentration. Lastly, verification and evaluation of the model's air quality estimates requires a suitable data base of measured air quality for comparison. Because existing monitoring networks are generally not designed to provide boundary conditions, initial conditions or adequate verification data, supplementary monitoring is usually required.

1. Requirements for Air Quality Data

As indicated in Table III-4, air quality data are needed to establish boundary conditions and initial conditions for model application and to verify the model results. The pollutants of primary concern are ozone and its precursors: nitrogen dioxide, nitric oxide, and nonmethane hydrocarbons. In addition, the composition of nonmethane hydrocarbons in terms of individual organic species is needed. Data for other pollutants, i.e., carbon monoxide, are of secondary importance only.

The monitoring data base should characterize the following aspects of the photochemical oxidant problem:

Table III-4

Air Quality Data Needs

Boundary Conditions	Ground-level concentrations on upwind boundary of region, concentrations aloft, and temporal variation of O_3, NO_2, NO and NMHC.
Initial Conditions	Early morning ground-level concentrations throughout region, concentrations aloft, and vertical profiles of O_3, NO_2, NO, and NMHC.
Verification Data	Hourly ground-level concentrations of O_3 downwind and within urban area.
Miscellaneous Data*	Species composition of NMHC aloft and on the ground upwind and within urban area; concentrations of CO. at existing monitors.

*Used to enhance both boundary conditions and initial condition data.

1. Ozone and precursor concentrations transported into the urban area from upwind source regions.

2. Precursor concentrations within the urban area as a result of local emissions.

3. Ozone concentrations within the urban area.

4. Maximum ozone concentrations downwind of the urban area.

The first two aspects need to be characterized in order to specify the initial and boundary conditions for input to the model. The third and fourth provide a basis for evaluating the model's estimates of ozone concentrations. Ozone concentrations downwind are of concern because this is where maximum ozone levels generally occur. Ozone levels within the urban area are also of concern because this is where population exposures are typically the greatest. In addition, precursor concentrations within the urban area are useful for evaluating the model's estimates of hydrocarbon and nitrogen oxide concentrations.

2. Collection of Air Quality Data

The data collection program should be designed on the basis of the upwind, urban, and downwind considerations just described. The siting of additional monitors is almost always required. Before supplemental monitoring stations are installed, however, existing stations and instrumentation should be used to best advantage. Relocation of existing stations should be considered if this will improve the monitoring network. Typically the data collection effort lasts three months, chosen to coincide with the "oxidant season." Historical ozone/oxidant data should be consulted, although the highest ozone levels generally occur between June and September in most regions of the United States.

The number and location of upwind (and downwind) monitoring stations depends on the consistency of the wind flow from any particular sector during high ozone periods. Historical records of air quality and meteorology should be examined to identify any prevailing wind directions on days with high measured ozone concentrations. The time of day should be considered in this regard since early morning surface winds tend to be light and variable whereas mid-day winds are more uniform and better represent the regional air flow pattern. If a single wind direction quadrant is identified, one or two upwind monitoring stations will probably suffice; otherwise more may be required. The monitors should be located fifteen to thirty kilometers upwind of the edge of the metropolitan area and be sited so as to avoid the effects of any localized emission sources, including highways. Ozone, nitric oxide, nitrogen dioxide, and nonmethane hydrocarbons should be measured at each upwind station.

Urban monitoring stations should be located so as to characterize the spatial distribution of ozone and precursors in the metropolitan area. The number of stations depends on the area's size and the configuration of its emission sources. At least two stations should be located in the central business district. Other sites should be selected so as to achieve a balanced representation of the emissions in the metropolitan area and to monitor areas of special interest (urban residential, suburban, or industrial areas, for example). The total number of urban sites may range from as few as three to as many as nine. Again, ozone, nitric oxide, nitrogen dioxide, and nonmethane hydrocarbons should be measured at each urban site.

Additional ozone monitors should be located downwind in order to determine ozone maxima under conditions of downwind transport. Their number and location depends, as for upwind monitors, on the existence of a predominant wind direction during periods of high ozone concentrations. Ozone maxima frequently occur fifteen to thirty kilometers or more downwind of the urban core. The total number of downwind stations may range from as few as four where the wind direction is highly persistent to as many as nine or more where it is not. At least one station should be located beyond the expected area of maximum ozone impact to assure that the network actually encompasses the highest values. Downwind stations should be sited away from areas of significant emissions, including isolated point sources and highways. If ozone levels in downwind suburban towns or cities are desired to be measured, additional stations would be needed.

If nitrogen dioxide is now or is expected to be a problem, additional instrumentation at the downwind stations nearest the urban area should be considered. Some evidence indicates that maximum nitrogen dioxide levels may occur five to fifteen kilometers downwind of the urban core.

In addition to the basic monitoring network, individual organic species should be measured in order to determine the ambient mix of carbon-bonds. Generally grab samples are taken over a three hour period and then analyzed in the laboratory by gas chromatography for species concentrations. The species data totals also serve as a check on the nonmethane hydrocarbon measurements. Grab samples should be taken at the urban monitoring stations and if transported hydrocarbons are expected to be significant, at the upwind stations as well.

Figure III-3 shows an air quality monitoring network for a major metropolitan area having a well-defined predominant wind direction from the west and southwest. In this case, the number of upwind, urban, and downwind stations is 2, 7, and 7, respectively. Ozone is measured at all 16 sites while NO_x and NMHC are measured both upwind and within the urban area. Due to the general urbanization of the area as a whole, NMHC is also measured

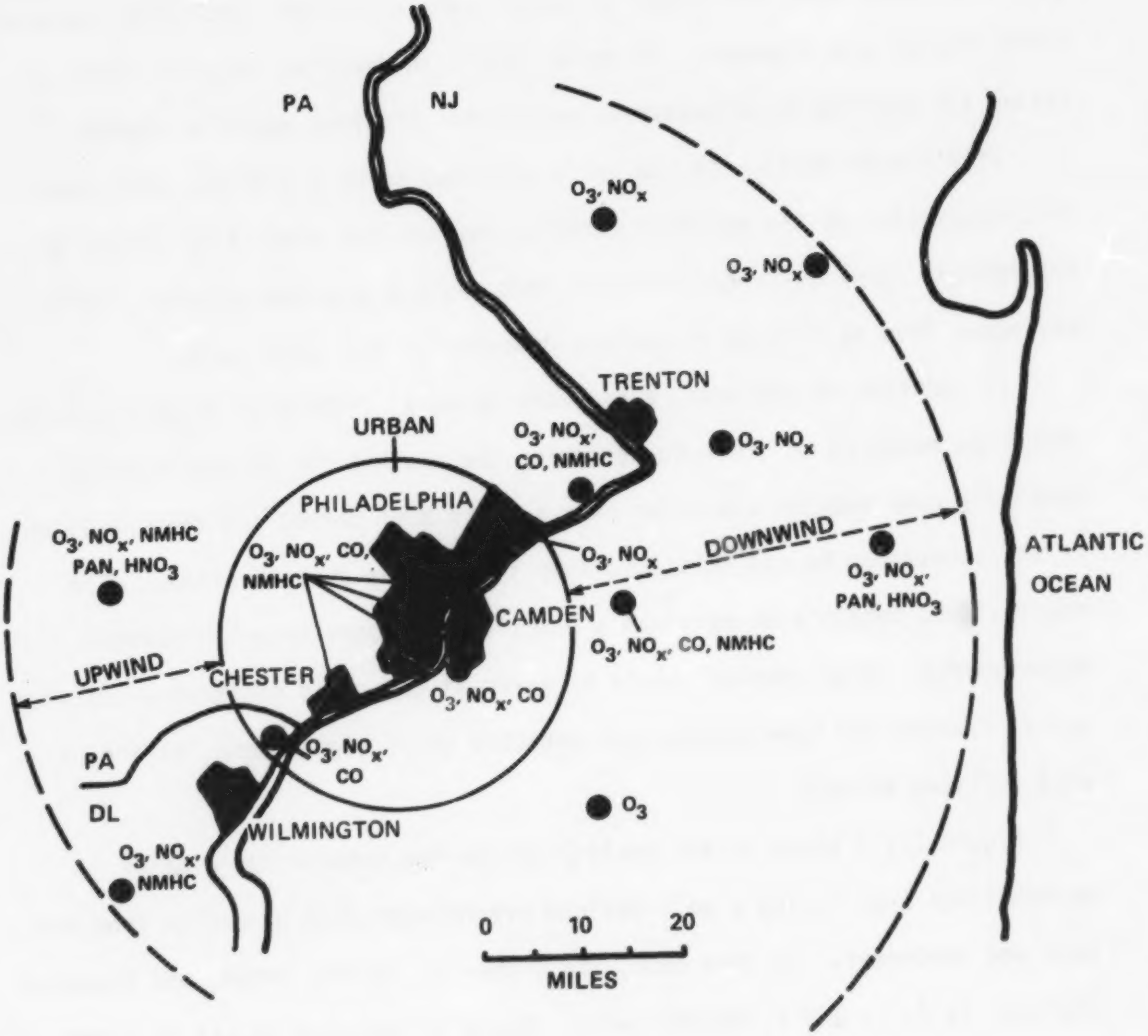
PA
NJ
O_3, NO_x
O_3, NO_x
TRENTON
URBAN
O_3, NO_x, CO, NMHC
O_3, NO_x
PHILADELPHIA
O_3, NO_x, NMHC PAN, HNO_3
O_3, NO_x, CO, NMHC
O_3, NO_x
DOWNWIND
ATLANTIC OCEAN
O_3, NO_x, PAN, HNO_3
CAMDEN
O_3, NO_x, CO, NMHC
UPWIND
CHESTER
O_3, NO_x, CO
O_3, NO_x, CO
PA
DL
O_3
WILMINGTON
O_3, NO_x, NMHC
0
10
20
MILES

Figure III-3. An Air Quality Monitoring Network for Philadelphia.

at two near downwind locations while NO and NO_2 is recorded both near and far downwind. In this example, several other pollutants are measured which are not always included in a photochemical monitoring program. These are HNO_3, PAN, and CO. The nature of the monitoring network for any particular city will depend on local factors, including the size of the urban area, the location of existing monitors, the importance of inter-urban transport, and the prevailing wind direction(s) during periods of high ozone concentrations.

Development of a monitoring data base imposes quality assurance requirements more stringent than for routine monitoring purposes. Site exposure should be in conformance with established guidelines (Ludwig and Shelar, 1978). Routine instrument checks, including zero and span, should be performed twice per week during the three-month study period and independent audits should be performed once a month. These quality assurance measures should be conducted at both the existing and supplemental monitoring stations.

When transport of ozone and precursors into an urban area is known or suspected to be significant, air quality measurements aloft are desirable. Instrumented aircraft equipped with ozone and nitrogen oxide/nitric oxide monitors are generally used. Grab samples should also be collected in order to characterize the organic species mix aloft. Aircraft measurements are usually limited to days on which high ozone levels are expected.

C. METEOROLOGICAL DATA

As stated earlier, the Airshed Model simulates the urban atmosphere under the constraint that pollutant mass is conserved. Conservation of mass requires that pollutant transport through the faces of each grid cell be known or estimated. This includes both advection in the horizontal and dispersion in the vertical. Advection is defined by the time-averaged wind vector while dispersion is related to fluctuations in the wind and to vertical turbulence. Variations in the vertical distribution of temperature affect the vertical extent of mixing within a column of grid cells. The height to which the mixed layer extends is termed the mixing height. In order to simulate all these processes, a three-dimensional wind field and a two-dimensional field of mixing heights, as well as atmospheric stability, all as a function of time, are required.

Another important meteorological parameter is solar insolation since several key photochemical reactions are driven by sunlight. The amount of insolation present, as a function of time, must therefore be known or estimated.

1. Requirements for Meteorological Data

Meteorological data needed to characterize the wind field, mixing height, stability, and solar insolation are listed in Table III-5. Hourly surface observations of wind speed and wind direction are necessary to describe pollutant transport at the surface while vertical profiles of speed and direction at various times during the day are necessary to describe the upper-level winds. Measurements of vertical temperature gradients at various times are used together with hourly air temperatures at the surface to estimate hourly mixing heights. Vertical temperature gradients are also used (along with solar insolation data) to characterize atmospheric stability within the mixed layer.

In order to adjust the photochemical rate constants so as to reflect the amount of radiation available, solar insolation measurements are

Table III-5

Meteorological Data Needs

Wind Field	Hourly surface observations of wind speed and direction throughout region; vertical profiles of wind speed and direction and their temporal variation.
Mixing Height and Stability	Hourly surface temperature observations throughout region; vertical temperature gradients and their temporal variation.
Miscellaneous Data	Hourly surface observations of solar insolation; surface observations of relative humidity and pressure and their temporal variation.

needed. Surface air temperatures are also used to adjust various chemical reaction rate constants. Observations of relative humidity are needed in order to compute water vapor concentrations which in turn enter into the photochemistry of oxidant formation (though the effect is minor). Conversion of pollutant concentrations from a mass to a volume basis requires that atmospheric pressure be known.

2. Collection of Meteorological Data

The number of meteorological monitoring stations needed is related to the size of the city and the complexity of the wind field. Metropolitan areas located adjacent to coastlines or lakeshores and areas located in complex terrain will require special consideration when designing the meteorological monitoring program. As discussed in Chapter IV, Preparation of Model Input Data, wind field modeling may be required in such situations. The wind data collection effort would then be directed at satisfying the needs of the model chosen. Even for inland areas having relatively flat terrain, significant heat island effects may be encountered. Sufficient spatial resolution is required to characterize these effects. Meteorological data collection should occur over the same three month period as the air quality monitoring. The following discussion of requirements is applicable to metropolitan areas with generally flat terrain and minimal sea breeze effects.

In general, wind instrumentation should be collocated with the air quality monitoring stations discussed previously. The upwind, urban, and downwind nature of the regional air flow can therefore be characterized and upwind-downwind trajectories can be determined. However, care should be taken to insure that wind instruments are sited to avoid microscale wind effects such as may be experienced in the lee of buildings or in close proximity to topographic features. Depending on city size and configuration, as well as factors mentioned previously, the minimum required number of upwind stations may range from one to three, urban stations from two to five, and downwind stations from two to four in number. Wind instruments at existing air quality monitoring stations should be incorporated in the study network if possible. National Weather Service wind data, which is usually collected at major airports and should be available in most all metropolitan areas, can be used to further supplement the wind monitoring network.

Mixing heights are oftentimes determined by measuring the vertical temperature gradient in the atmosphere. Although twice daily mixing heights are routinely available from the National Weather Service in many metropolitan areas, the measurements are normally taken in rural rather than urban settings. These data should therefore be supplemented with additional radiosonde ascents and surface temperature measurements in order to characterize mixing heights over the modeling region and their variation with time. In particular, estimates are needed of the minimum mixing height before sunrise, the mixing height during the mid-morning when the rate of rise is quite rapid, and the maximum mixing height in the afternoon. A minimum of three ascents each day should be made at an urban site with release times of 0400, 1000, and 1500, for example. Upwind of the city, the primary concern is the development of the mixing layer after sunrise. Therefore, radiosonde releases should also be conducted at an upwind site at 0500 and 0900, for example. Alternatively, an acoustic sounder may be an advantageous and economical method of obtaining morning mixing heights at the upwind site. (However, if an acoustic sounder is used, an additional pibal site should be added to those suggested below.)

If aircraft flights are conducted to measure pollutant concentrations aloft, the aircraft should be equipped with temperature sensors to further define the temperature structure of the atmosphere. In addition, since surface temperature measurements can be used to help interpolate mixing heights temporally and spatially, such measurements should be taken at the wind monitoring stations discussed previously.

The radiosonde ascents should be supplemented with pibal ascents in order to characterize air flow aloft. By tracking the pibal or radiosonde over time, vertical profiles of wind speed and wind direction can be inferred. Generally two or three pibal release sites are desirable. The locations and times of their release should be coordinated with the radiosonde ascents so as to provide a maximum overall representation of the regional wind field.

Solar insolation (both direct and diffuse) is readily measured using a pyranometer. The number of sites depends on the size of the city, and the presence of water or terrain which might influence cloud cover. In general however, two monitoring sites are desirable. The instruments should be collocated with the wind and air quality instrumentation at stations representative of upwind, urban, or downwind locations.

In regard to relative humidity and atmospheric pressure, no additional data need normally be collected. National Weather Service or local agency surface measurements, normally taken every hour, are generally sufficient for modeling purposes.

Figure III-4 shows a meteorological monitoring network for a major metropolitan area having a well-defined predominant wind direction from

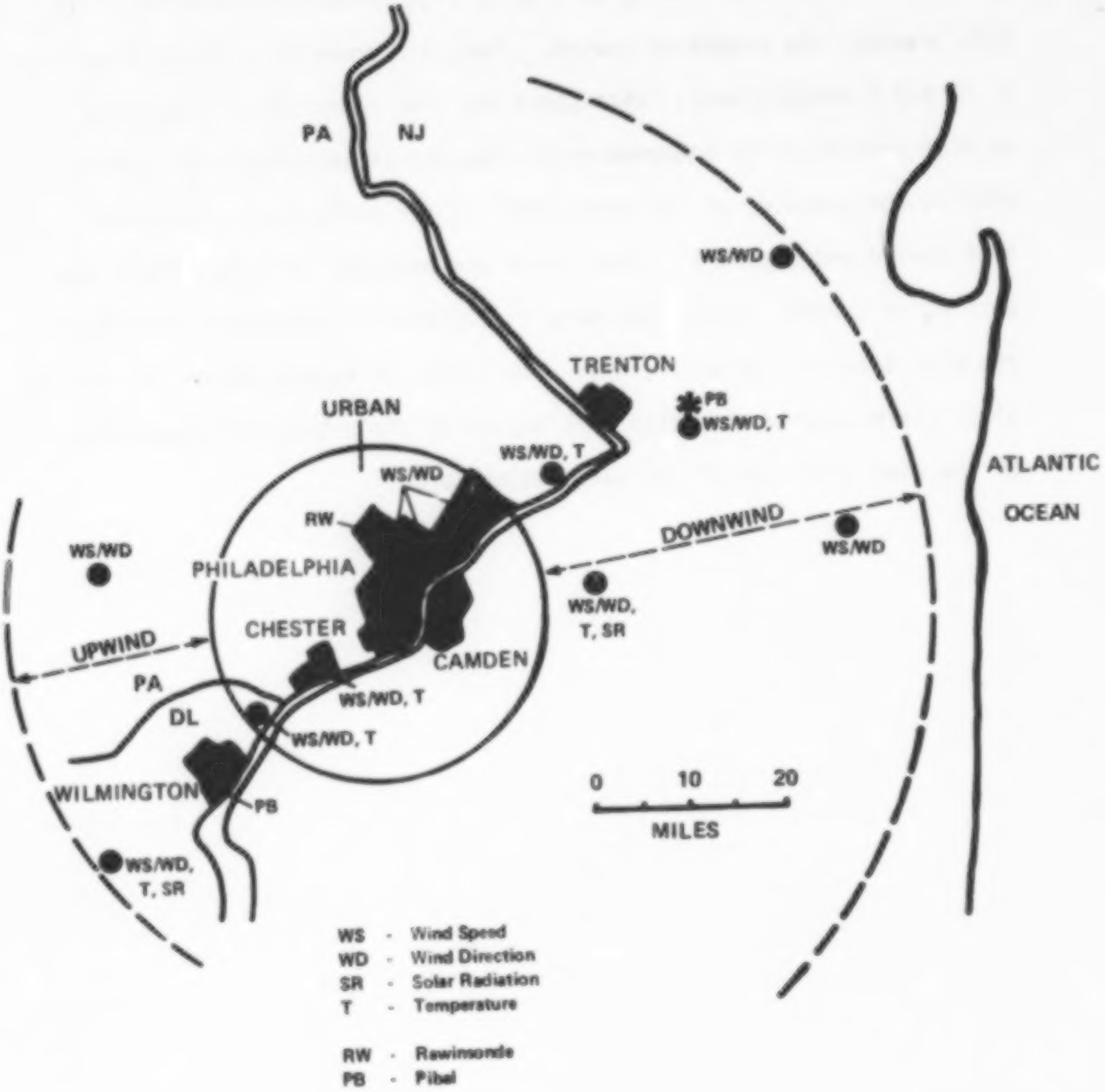
PA
NJ
WS/WD
TRENTON
PB
WS/WD, T
URBAN
WS/WD, T
WS/WD
ATLANTIC
OCEAN
RW
DOWNWIND
WS/WD
WS/WD
PHILADELPHIA
WS/WD,
T, SR
CHESTER
UPWIND
CAMDEN
PA
WS/WD, T
DL
WS/WD, T
0
10
20
MILES
WILMINGTON
PB
WS/WD,
T, SR
WS - Wind Speed
WD - Wind Direction
SR - Solar Radiation
T - Temperature
RW - Rawinsonde
PB - Pibal

Figure III-4. A Meteorological Monitoring Network for Philadelphia.

the west and southwest during periods of high ozone concentrations. In this example, the number of upwind, urban, and downwind surface sites is 2, 5, and 5 respectively. Wind speed and wind direction are measured at each station while temperature is recorded at selected sites upwind, within, and downwind of the urban area. Solar radiation is measured both upwind and downwind. Winds aloft are measured at three sites, one each at an upwind, urban, and downwind location. Temperature soundings are also taken at the urban site. The number of meteorological monitoring sites for any particular city will depend on the nature and complexity of the wind field and of the surrounding terrain.

CHAPTER IV. PREPARATION OF MODEL INPUT DATA

Once the emissions, air quality, and meteorological data described in Chapter III have been assembled, the data must be prepared for model input. Data preparation includes selection of a set of individual modeling days from the meteorological and air quality data bases for which model input data is to be prepared. Once the data has been prepared, the model can be run. Model operation is described in detail in the User's Manual for the Airshed Model* (Ames, et. al., 1978) and will not be discussed here. Computer resources necessary to run the model are, however, described briefly in Chapter VI, Resource Requirements for an Airshed Model Application.

A. DAY SELECTION CRITERIA

Prior to attempting to prepare the aerometric data for model input, one must select the days to be modeled. Normally, three or four days should be selected. Several selection criteria should be observed. First, ozone levels should be near the maximum that occurred during the air quality monitoring program. Such high ozone episodes often occur over a two or three-day period. Second, weekend days should be avoided. Use of an emission inventory developed for a weekday may introduce errors if used on a weekend day. Total regional emissions are lower on weekends and the temporal and spatial distribution of the emissions are different. Third, the aerometric data base should be relatively complete. Excessive occurrences of missing data makes data preparation difficult and may lead to a poor or suspect verification. Fourth, the air quality and meteorological data should not exhibit abnormal complexity. Unusual wind fields or concentration gradients may place undue stress on the model. Such occurrences may cause the data itself to be suspect in some cases. Passage of warm or cold fronts may introduce unacceptable complexities. Under no circumstances should any precipitation have occurred during the pre-dawn to mid-afternoon hours. In general, sunny skies and light winds associated with slow-moving high pressure systems are conducive to high ozone levels.

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*At this time, only a draft has been provided by Systems Applications, Inc. The manual will be available for public release upon completion of a finalized version.

B. DATA INPUT FILES

The Airshed Model contains eleven data preparation programs which assist the user in creating the aerometric and emissions input files required for a simulation run. Figure IV-1 shows the input data files while Table IV-1 provides a short description of each. A variety of alternate methods for preparing the aerometric data are possible. Selection of a method depends on the nature of the data base. The level of sophistication of the method selected follows from the level of sophistication of the data base. Several methods depend upon interpolation/extrapolation routines in the horizontal using station measurements. Vertical resolution is generally specified by means of normalized vertical profiles. Different methods may be used for preparing the data for different subregions. This allows the modeler to better utilize a spatially uneven data base as well as characterize spatial differences more realistically. Table IV-2 indicates the spatial and temporal resolution for each data input parameter that is achieved by utilizing the preparation programs.

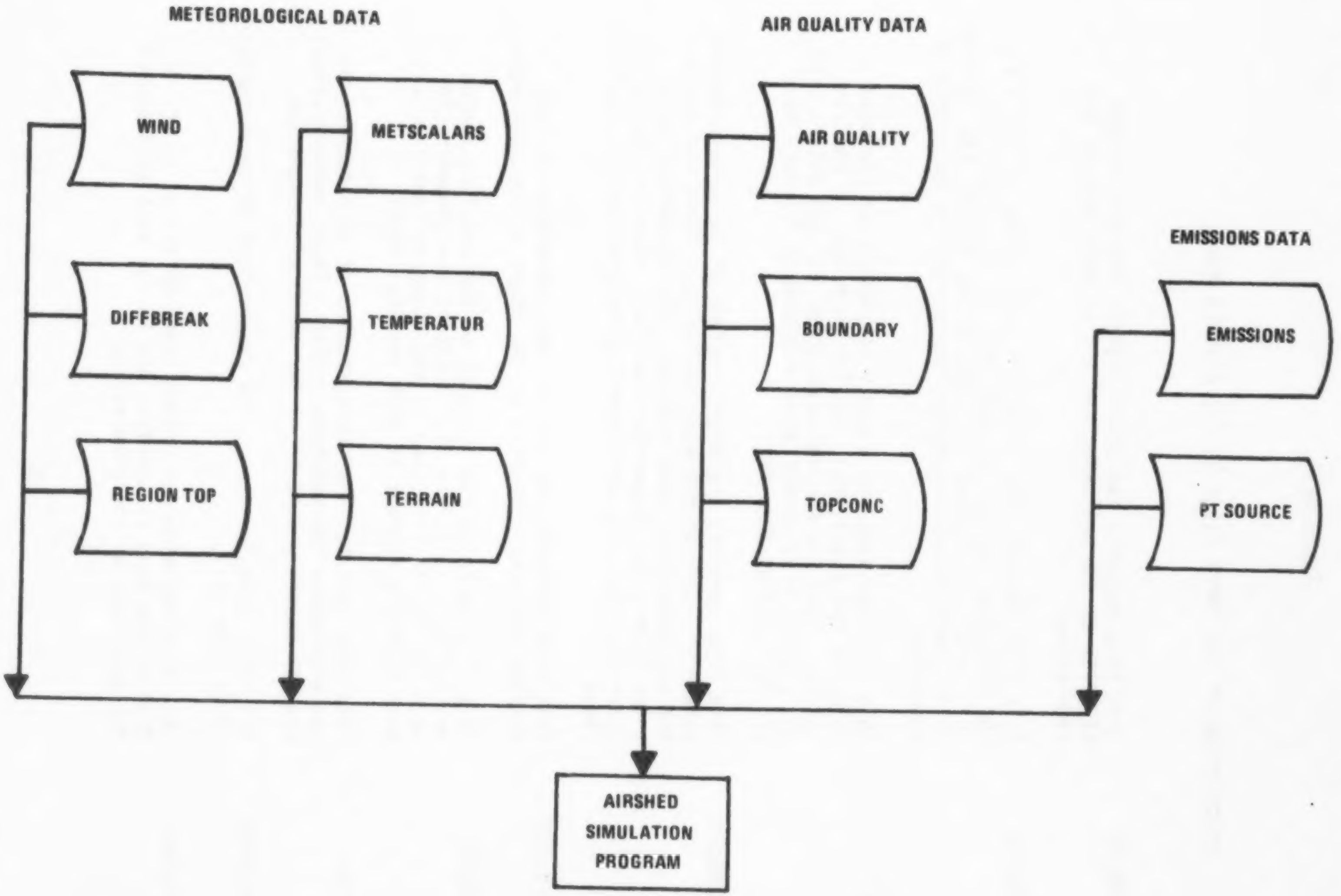

METEOROLOGICAL DATA
WIND
DIFFBREAK
REGION TOP
METSCALARS
TEMPERATUR
TERRAIN
AIR QUALITY DATA
AIR QUALITY
BOUNDARY
TOPCONC
EMISSIONS DATA
EMISSIONS
PT SOURCE
AIRSHED
SIMULATION
PROGRAM

Figure IV-1. Input data files for airshed simulation program.

Table IV-1.

DESCRIPTION OF THE INPUT FILES TO THE AIRSHED MODEL

DIFFBREAK	This file contains the mixing height for each column of cells at the beginning and end of each hour of the simulation.
REGIONTOP	This file contains the height of each column of cells at the beginning and end of each hour of the simulation. If this height is greater than the mixing height, the cell or cells above the mixing height are assumed to be within an inversion.
WIND	This file contains the x and y components of the wind velocity for every grid cell for each hour of the simulation. Also the maximum wind speed for the entire grid and average wind speeds at each boundary for each hour are included on this file.
METSCALARS	This file contains the hourly values of the meteorological parameters that do not vary spatially. These scalars are the NO_2 photolysis rate constant, the concentration of water vapor, the temperature gradient above and below the inversion base, the atmospheric pressure, and the exposure class.
AIRQUALITY	This file contains the initial concentrations of each species for each grid cell at the start of the simulation.
BOUNDARY	This file contains the location of the modeling region boundaries. This file also contains the concentration of each species that is used as the boundary condition along each boundary segment at each vertical level.
TOPCONC	This file contains the concentration of each species for the area above the modeling region. These concentrations are the boundary conditions for vertical integration.
TEMPERATUR	This file contains the hourly temperature for each surface layer grid cell.
EMISSIONS	This file contains the ground level emissions of NO, NO_2, five carbon bond categories, and CO for each grid square for each hour of the simulation.

Table IV-1. (Continued)

PTSOURCE	This file contains the point source information, including the stack height, temperature and flow rate, the plume rise, the grid cell into which the emissions are emitted, and the emissions rates for NO, NO_2, five carbon bond categories, and CO for each point source for each hour.
TERRAIN	This file contains the value of the surface roughness and deposition factor for each grid square.

Table IV-2

DATA-RELATED INPUT PARAMETERS FOR THE AIRSHED MODEL

Description	Spatial and Temporal Resolution*			Remarks
	xy	xyz	t	
METEOROLOGY				
Horizontal (u-v) winds (m/sec)		x	x	The vertical component, w, is computed by the Airshed Model, rendering the resultant wind field mass consistent
Reference height of surface wind monitoring stations (m)	x			Used in the diffusivity algorithm
Diffusion break (m)	x		x	Elevation at which the stability structure of the atmosphere changes markedly (e.g., an inversion or thermal internal boundary layer)
Top of modeling region (m)	x		x	Generally defined in relation to diffusion break
Ground-level temperatures (°C)	x		x	Used in kinetic module
Surface atmospheric pressure (mb)			x	Used in computing grid cell concentrations associated with emissions
Temperature gradient below diffusion break (°C/m)			x	Used in plume rise calculations
Temperature gradient above diffusion break (°C/m)			x	Used in plume rise calculations
Water concentration in the atmosphere (ppm)			x	Used in kinetic module
Exposure (stability class)			x	Used in diffusivity algorithm
Radiation intensity factor (per min)			x	Used in kinetic module
Surface roughness (cm)	x			Used in diffusivity and surface sink algorithms

Table IV-2 (continued)

	Spatial and Temporal Resolution*			
Description	xy	xyz	t	Remarks
Vegetation factor	x			Used in surface sink algorithms
AIR QUALITY				
Initial conditions (pphm)		x	x	Required for NO, NO_2, O_3, five carbon bond categories, PAN, BZA, and CO
Boundary conditions (pphm)		x	x	Required for same pollutants as above
Concentrations above top of modeling region (pphm)	x		x	Required for same pollutants as above
EMISSIONS				
Lumped ground-level emissions from stationary and mobile sources (gm-moles/hr)	x		x	Required for NO, NO_2, five carbon-bond categories and CO
Elevated stationary point source emissions (gm-moles/hr)		x	x	Emissions from tall stacks for the above pollutants are required
Elevated point source stack data including height (m) temperature (°K) diameter (m) and velocity (m/sec)	x			Used in plume rise calculations

*xy indicates two dimensional data field
xyz indicates three dimensional data field
t indicates time varying data field

1. Preparing the Meteorological Data

Preparation of the METSCALAR and TEMPERATUR input files is relatively straightforward. The METSCALARS file contains those meteorological parameters which do not vary spatially. Hourly values of the average temperature gradient below and above the mixing height and hourly values of atmospheric pressure, water concentration (derived from humidity measurements), and exposure (stability) class must be specified. In addition, hourly NO_2 photolysis rate constants must be input. The latter are readily calculated using measured solar insolation and estimated solar angle (Schere and Demerjian, 1978). Preparation of the TEMPERATUR file requires that hourly station temperature readings must be input and the desired interpolation routine selected.

Preparation of the DIFFBREAK file generally requires the use of algorithms or techniques external to the data preparation program. Vertical temperature gradient readings (2 to 3 sites, 3 to 4 times daily) and surface temperature readings (5 to 12 sites, hourly) are used to determine hourly mixing heights at all stations (7 to 15 sites). These values are then input to the data preparation program and a suitable spatial interpolation routine is selected. Creation of the REGIONTOP file does not involve any actual data input. Rather, the user generally specifies the number and height of grid cells above the mixing height. Alternatively, a fixed region height may be used.

Preparation of the WIND file requires special expertise in wind field modeling and analysis and the use of specialized wind generation programs. Such programs are not provided by the Airshed Model. The WIND file should be recognized as a critical element of satisfactory model performance. For these reasons, the WIND file is undoubtedly the most challenging file to prepare. An iterative procedure, whereby wind field modeling is conducted and the resulting wind field is evaluated, is usually necessary.

Three distinct approaches toward generating wind field inputs may be taken. The simplest approach is the use of an interpolation scheme whereby station readings of wind speed and wind direction are used to approximate values in each grid cell. Vertical wind profiles derived from pibal, rawinsonde, or other measurements, are also used. The interpolation scheme must be followed by a smoothing of the resulting multilayer, horizontal wind fields. This is necessary to reduce divergence in the resulting wind field. The Airshed Model simulation program itself then removes any remaining divergence by generating compensating vertical winds, thus insuring a mass consistent wind field.

An alternative and more sophisticated approach is the use of so-called "diagnostic models." Such models are appropriate where the local terrain configuration has a significant effect on wind patterns. These models, which incorporate some of the same concepts discussed above, use a basic conservation of mass equation subject to various boundary constraints. Such constraints may include heat island effects as well as terrain blocking and channeling effects and inversion limiting effects.

The most complex approach is a dynamic wind field model based on the solution of mass, momentum, and energy equations. These models may be needed in areas with significant thermally generated sea or lake breezes. Unfortunately, their data input requirements are considerable and their computer requirements are comparable with those of the Airshed Model itself.

A technique, which is available as an Airshed Model data preparation program, may be used in special situations where terrain and water effects are negligible and little wind data is available. It uses an average wind vector together with a network of station temperature readings to approximate urban heat island effects.

Preparation of the TERRAIN file involves the estimation of surface roughness and surface deposition factors throughout the modeling region. Pollutant uptake by water bodies and vegetative surfaces may influence ozone concentrations. Standard factors are used to represent uptake by various types of surfaces such as trees, grasses, water, and man-made materials. The relative composition of individual grid squares and/or subregional areas in terms of these surface types can be approximated using land-use maps and assumed mixes for each land use category. Surface roughness is employed by the model to characterize vertical dispersion near the ground. Land-use maps, topographic maps, and the surface types described above are used to determine the roughness controlling features so standard roughness length values can be selected. As with surface deposition, roughness lengths may be specified at the subregional level or at the grid square level depending on its spatial variability.

2. Preparing the Air Quality Data

Three files use air quality data: BOUNDARY, AIRQUALITY, and TOPCONC. Although each is created by a separate data preparation program, care should be exercised to assure the files are mutually consistent. For example, the vertical distribution of upwind boundary conditions should be consistent with the values used above the modeling region. Otherwise, an artificial discontinuity is introduced. Each file contains values for the eleven pollutants listed in Table IV-3.

Table IV-3

POLLUTANTS TREATED BY THE AIRSHED MODEL

Pollutant	Airshed Model Name
Ozone	03
Nitric Oxide	NO
Nitrogen Dioxide	NO2
Organics:	
Highly Reactive Double Bonds	OLE
Aromatic Rings	ARO
Single-Bonded Carbon Atoms	PAR
Carbonyl Bonds	CARB
Moderately Reactive Double Bonds	ETH
Carbon Monoxide	CO
Benzaldehyde	BZA
Peroxyacetyl Nitrate	PAN

The AIRQUALITY file contains the initial concentration of each pollutant in each grid cell at the start of the simulation. Prior to use of the preparation program, nonmethane hydrocarbon values at the upwind and urban stations for the first hour are converted into the five carbon bond categories using the organic species data from early morning grab samples. (This conversion step is discussed further in regard to emissions in the Appendix, Technical Description of the Airshed Model.) Then these values, along with values of ozone, nitric oxide, and nitrogen dioxide are specified for each station at which they were measured. A suitable (horizontal) interpolation routine is then selected, one for each pollutant. If aircraft spirals were used to collect upper-level early morning air quality data, a vertical profile for each pollutant and the location the spiral was flown is specified. If not, a simple vertical profile must nevertheless by chosen. For example, values at the ground might be extended up to the mixing height. Estimated values aloft (discussed below) could be used above the mixing height. When interpolating horizontally or specifying a vertical profile, the modeling region can be broken up into subregions. However, designation of subregions must be observed for all pollutants.

For carbon monoxide interpolation routines may be used with one-hour data from the existing monitoring network. Without data aloft, values could be assumed constant in the vertical. For those pollutants not measured during the monitoring program (BZA and PAN), typical reference values may be used (Ames, et. al., 1978).

The BOUNDARY file contains the hourly concentrations of each pollutant for each boundary cell. The region boundaries must be defined first, however. This is done by assigning line segments which completely enclose the region. A ground-level value for each pollutant is then input for each boundary segment each hour. Deriving these values from the air quality data base is mostly a matter of judgment. The prevailing wind direction each hour is used to determine which stations are upwind or downwind. Downwind boundary values are not important although they must be input. As for initial conditions, nonmethane hydrocarbons must be converted to five carbon bond categories. A normalized vertical profile must also be specified for each boundary segment for each pollutant. These can be varied through the day. The vertical profiles should be tied to the ground-level value and the value aloft. If aircraft data has been collected, profile preparation involves selecting suitable profile methods and preparing the profile data sets so as to make the best use of available data. Even if upper-level data have not been collected, a simple assumed profile must still be entered.

The TOPCONC file contains the hourly concentrations of each pollutant above the modeling region. If aircraft data have been collected the data are used to determine the concentrations aloft of ozone, nitrogen dioxide, and nitric oxide. The results of aircraft organic species grab samples are used to estimate the concentrations of the five carbon-bond categories. If the data show any significant spatial variation, this should be represented either by using an interpolation routine with so-called "station" readings or by specifying a value for each grid square across the top of the region. Significant temporal variations should also be taken into account. If no upper-level air quality data are available, values aloft may be estimated crudely by using the late morning air quality measurements at an upwind ground-level monitoring station. This method assumes that upwind ground-level concentrations are indicative of concentrations aloft upon dissipation of the nocturnal surface inversion. For those pollutants not measured either upwind or aloft during the monitoring program (CO, BZA, or PAN) typical reference values may be used (Ames, et. a., 1978).

3. Preparing the Emissions Data

As discussed in Chapter III, Data Needs, the emissions data base should consist of hourly gridded ground-level emissions from minor point sources, area sources, and mobile sources. Each of these three files should contain the emissions for eight pollutants: NO, NO_2, OLE, PAR, CARB, ARO, ETH, and CO. These three files must then be merged to create the EMISSIONS file required by the Airshed Simulation Program.

While the EMISSIONS file contains the ground-level emissions, the elevated point source emissions are contained on the PTSOURCE file. Preparation of this file involves specifying the location and stack parameters (height, diameter, velocity, and temperature) for each major point source, entering the hourly emissions of the eight pollutants for each source, and running the data preparation program provided. The data preparation program utilizes the meteorological input files described earlier to compute plume rise and then assign the point source emissions to individual elevated grid cells.

CHAPTER V. EVALUATION OF MODEL PERFORMANCE

Before a model is used for assessing alternate control measures for reducing ozone precursor emissions, one must demonstrate the ability of the model to estimate ozone concentrations satisfactorily. Such a verification on several high ozone days is desirable. By simulating several meteorological and air quality situations, model performance can be evaluated over a range of conditions conducive to ozone formation. Should verification attempts fail on one day, other days are still available for analysis. Also, control measures may be more or less effective depending on the level of pollutant transport and the mesoscale meteorological conditions. In addition, verification on multiple days allows control strategies to be tested under different conditions.

Normally, single day verifications should be conducted for at least 14 hours, usually from about 5:00 a.m. to about 7:00 p.m. Such a time span covers the morning emissions peak and the afternoon ozone peak should it occur late in the day. However, if downwind ozone monitors clearly show that ozone levels drop off much earlier in the day, the length of the simulation may be shortened.

A number of performance measures may be used to evaluate whether or not the model is performing satisfactorily. Normally, performance is evaluated separately on each verification day. Both graphical and statistical techniques are useful. Several techniques should be chosen because different ones measure different aspects of the model's performance. Some measure the model's performance at estimating peak concentrations, others measure spatial and temporal correlations, while still others measure the overall accuracy of the model results.

The U. S. Environmental Protection Agency has recently published two reports addressing the evaluation of model performance: Procedures for

Evaluating the Performance of Air Quality Simulation Models (Hillyer, Reynolds, and Roth, 1979) and Performance Measures and Standards for Air Quality Simulation Models (Hayes, 1979). The first report summarizes various issues and considerations pertaining to model evaluation studies. The second report, in part, presents a number of specific performance measures.

Comparisons of model-estimated concentrations and observed concentrations must be done cautiously. Obviously, instrument error is always a complicating factor. Beyond this, however, the observed value at best represents a concentration measured at a single point. In contrast, the estimated value represents an average concentration within a surface layer grid cell; gradients within a cell cannot be accounted for. The Airshed Model does perform an east-west and a north-south linear interpolation between the four closest grid cells to obtain a point estimate. The grid cell average value is used to represent the value at the centroid of the cell for the interpolation. This procedure does not, however, compensate for the fundamental difference between observed and estimated values. It only provides an objective method for comparing model results to measured concentrations. Clearly, the representativeness of the monitor site is a key factor. For example, model estimates of NO_x or CO that are much lower than monitor readings while at the same time ozone estimates that are significantly higher may indicate the monitor is being unduly affected by localized emission sources under certain meteorological conditions. These kinds of disparities point up the need for properly siting ozone monitoring equipment when setting up the ambient network discussed in Chapter III. In general, the observed concentrations are nevertheless assumed to be the "true values" when using performance measures to evaluate model results.

The following discussion presents a variety of performance measures, both graphical and statistical, which have been identified for use in evaluating model performance. The measures discussed here are not intended as recommendations, as further experience with a wide variety of measures in various applications is needed in this newly developing field.

A. GRAPHICAL TECHNIQUES

Scatter diagrams are one of the most common graphical methods of comparing observed and estimated concentrations. Normally the observed values are plotted on the abscissa on the same scale as the model estimates which are plotted on the ordinate. A 45 degree line through the origin then represents a perfect correlation. The distance of points from this line is a measure of the deviation while the clustering of points above or below is a measure of bias. As shown in Figure V-1 maximum values at each station, mean values over a certain time interval (or the entire simulation), or all hourly values at all stations may be visually compared in this way.

Time histories of observed versus estimated concentrations at individual stations may also be presented graphically as shown in Figure V-2. Such plots show whether the model estimates conform to the temporal patterns exhibited by the monitoring data and the extent to which model estimates are out of phase with actual values.

If the monitoring network is sufficiently dense, it may be possible to plot isopleths of the observed concentrations and compare these to isopleths of the model estimates, plotted at the same scale, as shown in Figure V-3. Two attributes may be examined using such plots: general pattern correspondence and directional alignment. General pattern correspondence is more important than simple directional alignment. Nonalignment may be caused

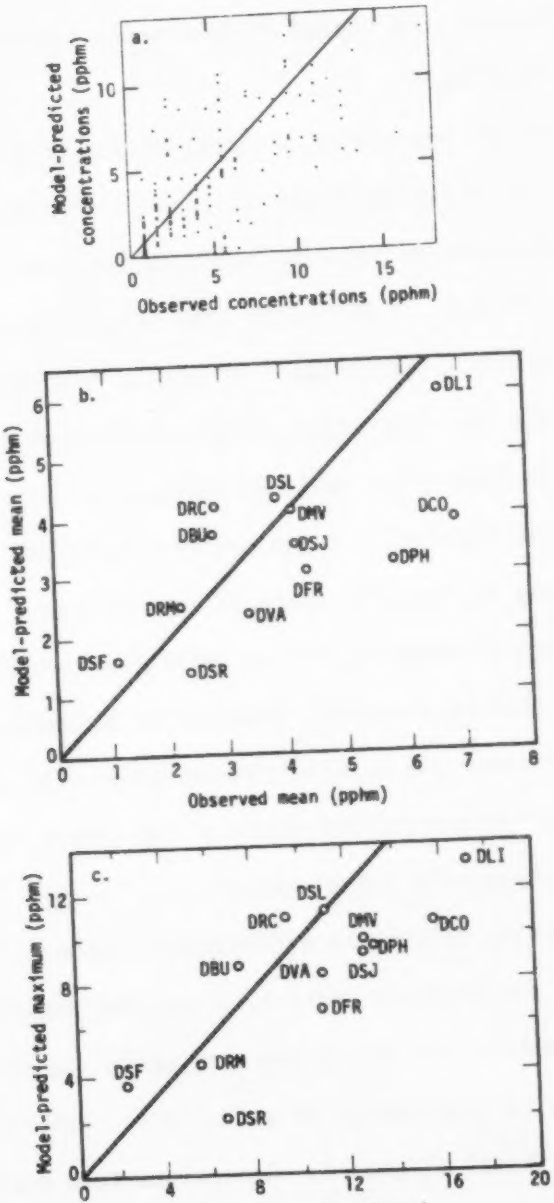


Figure V-1. Scatter diagrams of (a) observed oxidant concentrations versus calculated hourly average ozone concentrations, (b) observed versus calculated station mean concentrations, and (c) observed versus calculated station maximum concentrations (Duewer, MacCracken, and Walton, 1978).

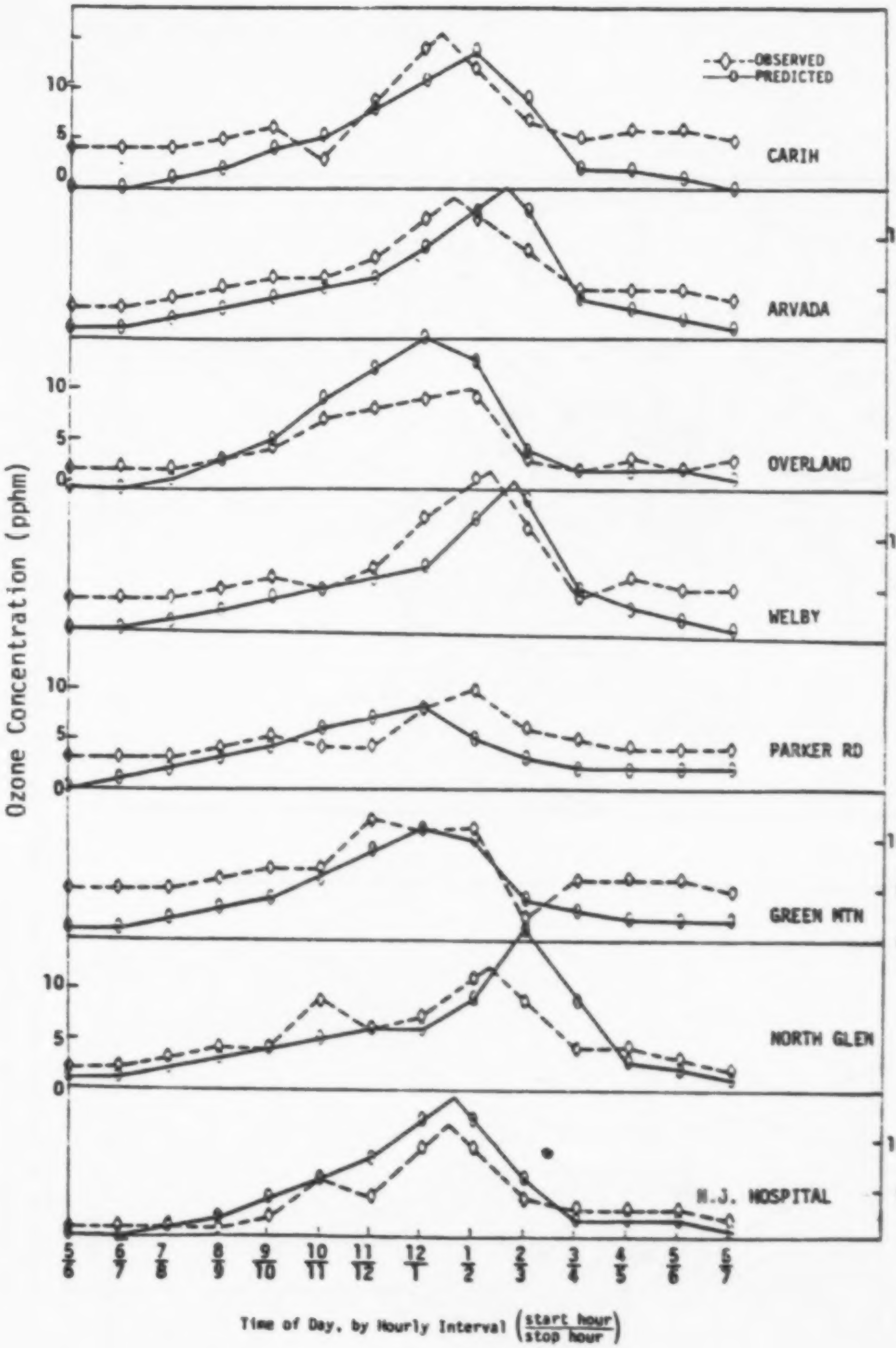
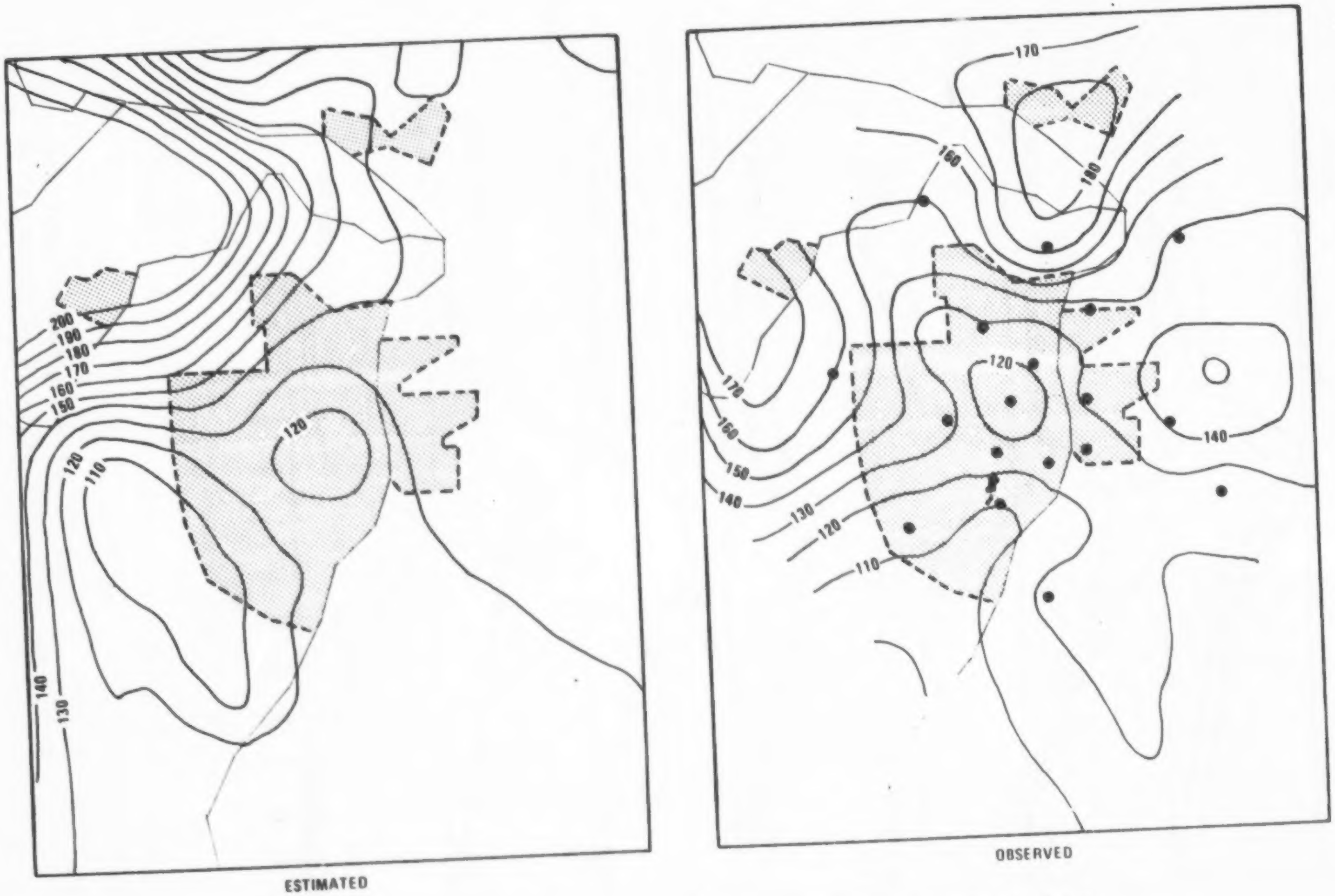


Figure V-2. Example of Plots Illustrating Model Predictions and Actual Measured Concentrations (Anderson, et al., 1977).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OBSERVED

Figure V-3. Comparison of estimated and observed ozone isopleths for the hour of maximum observed concentration.

by small errors in the wind field while a lack of pattern correspondence indicates a more fundamental problem with the data inputs or the model itself. Plots such as Figure V-3 may be further interpreted by comparing the areas over which ozone levels exceed certain threshold values above the standard.

B. STATISTICAL TECHNIQUES

As shown in Table V-1, a variety of numerical and statistical measures may be used for evaluating model performance. It is important to note at the outset that in most applications, the number of days modeled is insufficient to make any statistical statement regarding the ability of the model to estimate peak regional oxidant concentrations. Therefore it is not possible to say how the model might be expected to perform on a day other than those for which a verification analysis is actually undertaken.

The ability of the model to accurately estimate peak ozone concentrations is crucial to the application of the model for SIP planning purposes. The most obvious numerical measure is the difference between the estimated maximum ozone concentration at any station and the observed maximum ozone concentration at any station. This comparison is made irrespective of the time of day during which the maxima occurred. Another numerical measure of peak performance is derived by taking the ratio of the estimated maximum to the observed maximum concentration, one ratio for each station and then finding the median ratio. The median rather than the average value is used to avoid unnecessary bias that might be caused by a bad estimate at one or two stations, particularly at locations where both values are low.

Table V-1. Some Numerical and Statistical Performance Measures

Performance Attribute	Performance Measures
Accuracy of Peak Estimates	Difference between estimated and observed maximum concentration regardless of time or location
	Median ratio of estimated to observed maximum station concentrations
	Median relative absolute deviation between estimated and observed maximum station concentrations
	Correlation coefficient of estimated and observed maximum station concentrations
Overall Accuracy of Estimates	Median relative absolute deviation between estimated and observed station concentrations taken over all stations and all hours
	Average absolute deviation and standard deviation of absolute deviations between estimated and observed station concentrations taken over all stations and all hours
	Difference in the frequency of occurrence of values above some threshold, between estimated and observed station concentrations considering all stations and all hours
	Correlation coefficient of estimated and observed station concentrations taken over all stations and all hours
Absence of Bias	Relative deviation between estimated and observed maximum concentrations averaged over all stations
	Relative deviation between estimated and observed station concentrations averaged over all stations for hours when the observed value exceeds some threshold
Diurnal Pattern	Temporal correlation coefficient of estimated and observed station concentrations averaged over all stations
Spatial Pattern	Spatial correlation coefficient of estimated and observed station concentrations averaged over all hours

The median relative absolute deviation of maximum values, taken over all stations, times 100, is a good measure of the percent error associated with the peak ozone model estimate. The relative absolute deviation is defined here as the absolute value of the difference between the estimated and observed values, divided by the observed value. Another good statistical measure of peak model performance is the correlation coefficient, taken over all estimated/observed maximum concentration pairs, one pair for each station.

Because the intent of control strategy analysis is to reduce ozone concentrations below the standard and to reduce population exposure, it is also important that the model perform satisfactorily over a wide range of ozone concentrations. As with maximum concentrations, the median relative absolute deviation is also a measure of the overall percent error of the model estimates. In this case, however, rather than limiting the calculation to the maximum values, the median is taken using the entire set of deviations for all hours during the simulation. The overall correlation of all estimated and observed concentration pairs may also be computed. Measures of the absolute error and its variability are the average absolute deviation and the standard deviation of absolute deviations, respectively. The latter statistic involves the computation of the deviation of the absolute deviation of an estimated/observed pair from the average absolute deviation of all such pairs. Both statistics are computed over all stations and over all hours of the simulation.

A somewhat different performance measure involves the comparison of the cumulative frequency distribution of estimated ozone concentrations to the cumulative frequency distribution of observed ozone concentrations, again taken over all stations and all hours as in Figure V-4. A numeric comparison is then made of the frequency with which various concentration levels are exceeded.

One should also evaluate the model results for systematic bias. Bias occurs when the model has a tendency toward repeated errors in the same direction, either overestimation or underestimation. In this case, the algebraic average deviation rather than the absolute average is used. Normalizing the deviation by the observed concentration before averaging gives the average relative deviation, a measure on a fractional basis of the seriousness of the bias over any range of concentrations. Possible variations of this measure include restricting the computation to the maximum values for each station or to the hours during which the observed concentration exceeds some value, such as the ambient air quality standard. The overall bias may be assessed by extending the computation to include all stations and all simulation hours.

Quantitative statistical measures may also be used to evaluate the model's ability to generate satisfactory diurnal and spatial patterns. The temporal correlation coefficient, averaged over all stations, and the spatial correlation coefficient, averaged over all hours, are two such indices. Variations involve stratifying the data so that, for example, the temporal correlation is determined for stations individually or for groups of stations. Similarly, spatial correlations may be taken over one or more hours, usually the peak period.

C. REVERIFICATION

In the event of poor model performance, one must determine what is causing the model estimates to be unsatisfactory. The possible causes

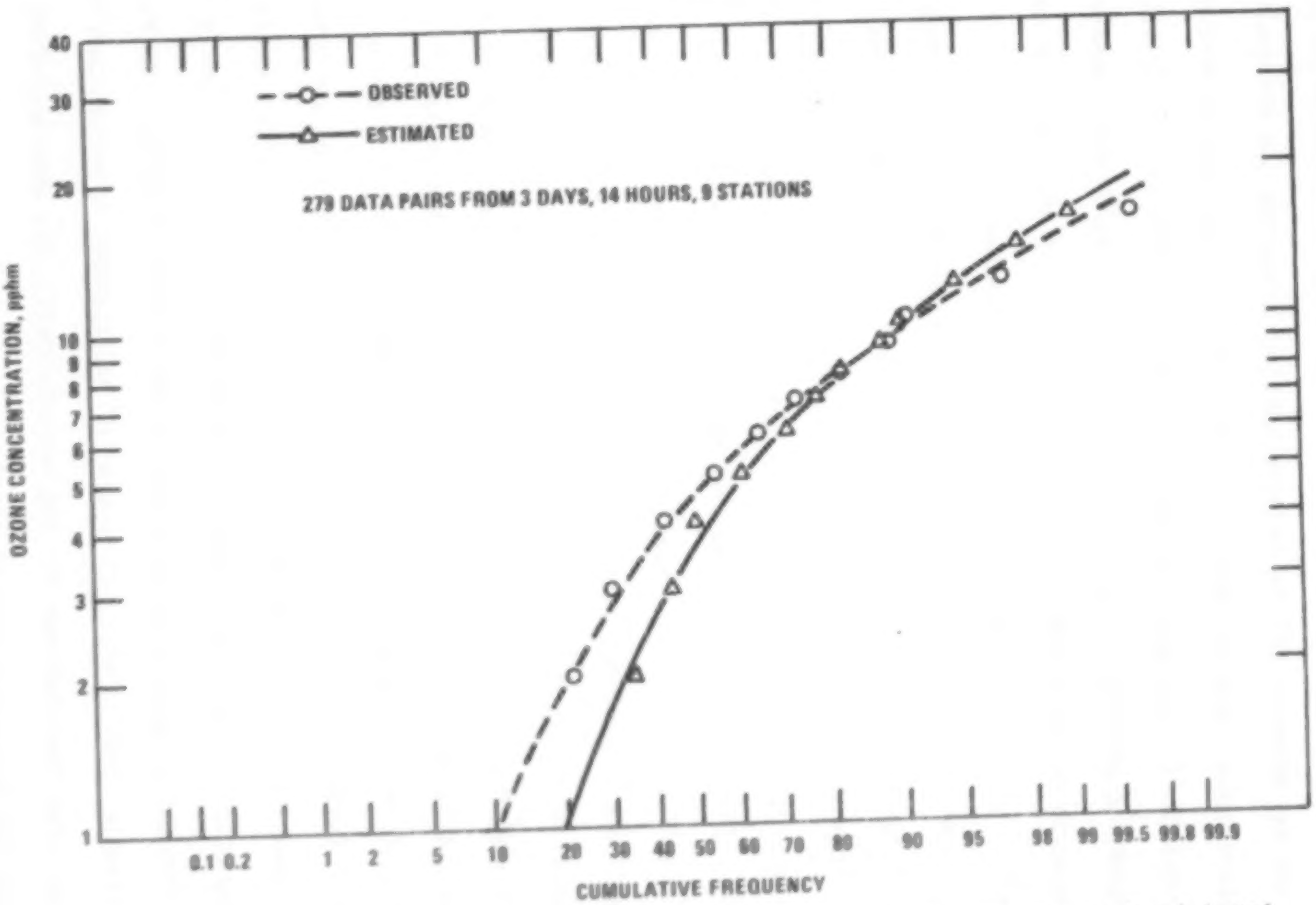

Figure V-4. Cumulative frequency distribution of estimated and observed ozone concentrations (adapted from Hayes, 1979).

may be grouped into three areas: (1) the emissions, air quality, or meteorological data bases may not adequately or properly characterize conditions on the day modeled; (2) the methods used for preparing the air quality and meteorological data for model input may not be appropriate or were exercised improperly; (3) the model may not be suitable or does not simulate the atmospheric phenomena important for the day or location being modeled. Unless a research and development type effort is being contemplated, one should probably not subject the last cause to any prolonged investigation. Rather, efforts should be placed on investigating the data base and improving and/or correcting the methods by which the data base was prepared for model input.

Generally, investigation of model performance problems should center initially on the procedures used for preparing the aerometric data for model input. This is because the modeler has the most control over this portion of the modeling study. Invariably, deficiencies exist in the data base which necessitate assumptions in order to prepare the data for the model. Such assumptions should be reevaluated. For example, preparation of the wind field and mixing height data are prime candidates for review. These two inputs are primary driving forces in the model simulation while the number of data points available and the methods used for their preparation methods may be less than ideal. Further analysis of the input data may improve model performance.

When investigating the data base, attention is most often focused on the emission inventory. This is due to the fact that emission inventories are frequently found to be deficient in one or more respects. One may find for example, that significant sources of hydrocarbons have been overlooked. One may also find that not all the vehicle traffic has been accounted for or that the input data used to compute mobile source emission factors is not representative or sufficiently resolved spatially and temporally. Another candidate for investigation is the organic species data used for allocating hydrocarbon emissions to the five carbon-bond categories. One might find for example that serious errors in judgment have been made in applying an imperfect organic species data base to specific sources in the inventory.

The modeler, due to his familiarity with the data base, the various methodologies, and their strengths and weaknesses should have a good idea of what areas warrant investigation and modification. Nevertheless, a knowledge of the sensitivity of the model to changes in input data is invaluable. For example, little is gained from expending much effort on reevaluating stability class data if the model results are not sensitive to stability class. While no comprehensive sensitivity study of the Airshed Model has been reported, Table V-2 summarizes the results of a number of sensitivity analyses performed with previous versions of the model and another photochemical grid model, the Livermore Regional Air Quality (LIRAQ) model. If all reasonable and objective modifications to the input data fail to upgrade model performance to a satisfactory level, then one is forced to admit that the model is unable to simulate the atmospheric conditions existing on that particular modeling day. In such cases, it is especially important that modeling of several different high ozone days has been provided for previously.

In summary then, model verification is not in any way a "push-button" operation. Rather, it is an iterative and an incremental process. With each execution of the simulation program model performance is evaluated, problems are diagnosed, the input data is reanalyzed, and the input files are modified until a satisfactory verification is achieved.

Table V-2 Summary of Sensitivity of Selected Photochemical Grid Models to Input Data Variations (Reynolds, Tesche, and Reid, 1978)

Study Group	Model Version and Attributes	Sensitivity Analysis Variations	Influence on Model Predictions	Remarks
MacCracken and Sauter (1975)	LIRAQ photochemical model Two-dimensional time-dependent grid model Lumped kinetic mechanism similar to Hecht-Seinfeld-Dodge mechanism Mass-conserving wind field	Relative humidity was reduced from 40% by 20%	Peak ozone increased by 3% and peak NO_2 decreased by 4%	LIRAQ sensitivity runs focused on the kinetic module; accordingly, sensitivity results are more reflective of smog chamber simulations than urban airshed simulations.
		Nominal temperature was increased from 285°K to 304°K	Peak ozone decreased by 2%, and peak NO_2 increased by 5%	
		Light intensity was reduced by 50%	Peak ozone decreased by 70%, and NO_2 peak magnitude remained unchanged but was delayed 4 hours	
		Light intensity was increased by a factor of 2	Peak ozone increased by 100%, and NO_2 peak magnitude slightly increased and preceded base case peak by 1-3/4 hours	
		Initial hydrocarbons were increased by a factor of 2	NO_2 peak increased by 6% and was delayed approximately 1 hour; ozone peak was not reported, but the increase in ozone concentrations was delayed by up to 3 hours	
		Initial NO_2 concentrations were increased by a factor of 2	NO_2 peak increased by 10% and was delayed slightly; O_3 remained unchanged	
Demerjian (1976)	SAI photochemical model: 1973 version	Boundary conditions were reduced by 50%	"Minor" differences occurred in ozone prediction in the eastern and northern portions of the L.A. basin; "significant" differences were observed in the western and central portions of the basin	
		Initial and boundary conditions were reduced by 50%	Predicted ozone in the northern and eastern edges of basin were reduced 20 to 30%	
Liu et al. (1976a)	SAI photochemical model: 1973 version 25 x 25 x 6 grid 15 step Hecht-Seinfeld-Dodge kinetics Price numerical method Empirical diffusion algorithm Two-dimensional wind field Two-dimensional initial conditions	Wind directions were randomly perturbed by 0 or ±22.5°	A 6.9% average deviation for manually prepared and 4.9% for automatically prepared wind fields (based on CO predictions) resulted	In the automatic wind field studies, perturbations were made to the monitoring station measurements and then automatic procedures were employed to derive gridded wind fields. In the manual wind field cases, perturbations were made to the gridded wind fields after they had been prepared manually.
		Wind speeds were randomly perturbed by 0 or ±1 mph	A 4.9% average deviation for manually prepared and 2.6% for automatically prepared wind fields (based on CO predictions) resulted	
		Wind station measurements were:	Maximum absolute deviation from the base case results for CO were:	The response of the model to variations in wind speed varies with each chemical species and is time dependent.
		Increased 50%	19.6%	
		Increased 25%	11.8%	
		Decreased 25%	20.2%	
		Decreased 50%	51.7%	

Table V-2 (Continued)

Study Group	Model Version and Attributes	Sensitivity Analysis Variations	Influence on Model Predictions	Remarks
		Horizontal diffusion was decreased to 0 and increased to 500 m^2/sec	For $K_H = 0$, the maximum absolute deviation for CO ranged between 0.52 and 2.02% from 0600 to 1600 hours For $K_H = 500$ m^2/sec, the maximum absolute deviation for CO ranged between 4.4 and 12.9% from 0600 to 1600 hours	
		Vertical diffusivity was decreased to 0.5 m^2/sec and increased to 50 m^2/sec	The effect of varying vertical diffusivity by an order of magnitude was about the same as that of varying the wind speed by 25 to 50%	The base case value was 5 m^2/sec.
		Mixing depths were increased and decreased by 25%	Maximum absolute percentage deviations for the increase and decrease, respectively, were: For CO, 8% and 12% For NO, 11% and 18.5% For NO_2, 8.5% and 15.5% For O_3, 11.5% and 23%	The buildup of the mixing depth variation effect is time dependent. Decreasing the mixing depth has a greater effect on the ground-level concentrations than increasing it; this result is more pronounced for reactive pollutants. The effect of changing the mixing depth is not uniform over the modeling region; it varies from place to place. The effect on ground-level concentrations of changing the mixing depth is roughly the same as that of changing the wind speed, as would be expected from a dimensional analysis.
		Radiation intensity was increased and decreased by 30%	Maximum absolute percentage deviations for the increase and decrease, respectively, were: For NO, 17% and 40% For NO_2, 74% and 55% For O_3, 9% and 11%	The effects of varying the radiation intensity are time dependent. The effect of changing light intensity is as significant as that of changing wind speed.
		Emissions rate (ground based) was increased and decreased by 15%	The effects of increasing and decreasing emissions rates are almost identical; peak basin-wide average percentage changes in CO and NO_2 were about the same (6-8%)	The study results are summarized by the following ranking of the relative importance of the input parameters (A = most important and D = least important):

Table V-2 (Continued)

<table>
<tr><th>Study Group</th><th>Model Version and Attributes</th><th>Sensitivity Analysis Variations</th><th>Influence on Model Predictions</th><th>Remarks</th></tr>
<tr><td></td><td></td><td></td><td></td><td><table>
<tr><th>Parameter or Variable</th><th>CO</th><th>NO</th><th>O_3</th><th>NO_2</th></tr>
<tr><td>Wind speed</td><td>A</td><td>A</td><td>A</td><td>A</td></tr>
<tr><td>Horizontal diffusivity</td><td>D</td><td>D</td><td>D</td><td>D</td></tr>
<tr><td>Vertical diffusivity</td><td>C</td><td>C</td><td>C</td><td>C</td></tr>
<tr><td>Mixing depth</td><td>B</td><td>B</td><td>B</td><td>B</td></tr>
<tr><td>Radiation intensity</td><td>D</td><td>A</td><td>A</td><td>B</td></tr>
<tr><td>Emissions rate</td><td>B</td><td>A</td><td>B</td><td>B</td></tr>
</table></td></tr>
<tr><td>Reynolds et al. (1976)</td><td>SAI photochemical model: 1973 version [see Liu et al. (1976a)]</td><td>Uniform wind velocities with height were compared with vertical variation in horizontal winds given by a power law formulation</td><td>The maximum average percentage deviations were: 28.5% for NO, 15% for NO_2, 24% for CO, and 14% for O_3
The maximum average deviations in pphm were: -0.35 for NO, -1.1 for NO_2, -4 for CO, and -2 for O_3
The maximum deviations in pphm were: 7.5 for NO, 15 for NO_2, 30 for CO, and 26 for O_3</td><td>The effects of including wind shear were similar to those of increasing surface wind velocities by roughly 25% because velocities within the mixed layer are increased between 20 and 70% of the surface values as a result of shear</td></tr>
<tr><td>Anderson et al. (1977)</td><td>SAI photochemical model: 1977 version
31 step carbon bond chemistry</td><td>Wind speeds were reduced by 33%</td><td>Maximum predicted ozone increased by 4%; maximum area for which $[O_3] \geq 0.06$ ppm increased by 12%</td><td></td></tr>
<tr><td></td><td>3-D wind field
Lower microscale layer</td><td>Mixing depths were reduced by 33%</td><td>Maximum predicted ozone increased by 16%; maximum area for which $[O_3] \geq 0.08\%$ ppm increased by 7%</td><td></td></tr>
<tr><td></td><td>Lamb and Liu diffusivity algorithms</td><td>Wind speeds and mixing depths were both reduced by 33%</td><td>Maximum predicted ozone increased by 33%; maximum area for which $[O_3] \geq 0.08$ ppm increased by 30%</td><td>A synergism exists between wind speed and mixing depth</td></tr>
<tr><td></td><td>30 x 30 x 7 grid
SHASTA numerical method
Surface removal
Three-dimensional initial conditions</td><td>Emissions in suburban areas surrounding Denver were reduced 25% with weighted emissions increases in other areas to make overall regional emissions equivalent to those in the base case</td><td>No difference occurred in the time, location, or magnitude of maximum ozone concentration; differences among predicted ozone concentrations in all runs were not more than 0.010 ppm in at most one or two grid cells</td><td>In each scenario, no more than 7% of the region-wide emissions were redistributed; changes of this size in the spatial distribution of emissions has little effect on secondary pollutants such as ozone</td></tr>
</table>

Table V-2 (Continued)

Study Group	Model Version and Attributes	Sensitivity Analyses Variations	Influence on Model Predictions	Remarks
		Emissions in the Denver metropolitan area were reduced 17.5% with a proportional increase in suburban areas to make regional emissions levels equivalent to those in the base case	No difference occured in the time, location, or magnitude of maximum ozone concentration; differences among predicted ozone concentrations in all runs were not more than 0.010 ppm in at most one or two grid cells	
Killus (1977) (private communication)	SAI photochemical model: 1977 version [see Anderson et al. (1977) for model attributes]	Grid spatial resolution was relaxed from 1 x 1 mile to 2 x 2 miles	The coarser grid resolution led to no noticeable change in the time to peak NO, NO_2, and O_3 concentrations; the magnitude of peak concentrations was reduced for NO (69%), NO_2 (21%), and O_3 (13%)	By the time ozone forms, its precursors have been distributed over a much greater area than their source regions; accordingly, the influence of increased grid size on ozone predictions should be less than that for primary pollutants such as NO
Anderson (1977) (private communication)	SAI photochemical model: 1977 version [see Anderson et al. (1977) for model attributes]	NO emissions from a point source were increased by 20% (note that the source contributes roughly 1% of the Denver regional NO_x burden)	The maximum impact of increased source emissions anywhere in the modeling region was an increase in hourly averaged NO and NO_2 concentrations (12 and 5 ppb, respectively) and a decrease in O_3 (-4 ppb)	The effect was decidedly local and did not influence peak oxidant concentrations

CHAPTER VI. MODEL APPLICATION FOR AIR QUALITY PLANNING

Model application refers here to the use of an air quality model to evaluate a specific air quality problem and to formulate control strategies which, when implemented, will ameliorate if not eliminate the problem. From a regulatory viewpoint, the question the model application phase attempts to address is: how much control is needed to reduce hydrocarbon emissions to a level at which the ozone standard is attained? An ancillary question is: what effect does nitrogen oxide control have on ozone levels? The air quality planner would also like to know, for a given overall regional emission reduction, what source categories are most effective to control and to what level. All of these questions can be addressed in an Airshed Model Application.

Before formulating control strategies, the air quality planner will want to know what the situation is likely to be in future years, in terms of ozone levels, if no additional controls are adopted. This is determined by applying the Airshed Model using the baseline projection emission inventories described in Chapter III. Data Needs. A preliminary estimate of the level of additional control needed can then be made.

Two approaches have been used to formulate candidate control strategies, one more rigorous than the other. The simpler approach is to use the Airshed Model in a so-called "sensitivity" mode whereby incremental across-the-board emission reductions are made and the resulting ozone concentrations are simulated. By employing this procedure, one attempts to "narrow in" on the overall emission reduction needed and to subsequently select the control measures necessary to provide that reduction. The preferred procedure is to simulate actual control measures in the context of an overall strategy. By simulating alternate strategies, an optimum strategy may be identified. Whichever approach is taken, the final set of control measures should be tested with the Airshed Model in order to demonstrate attainment.

A. PREPARATION OF FUTURE YEAR EMISSIONS

Whether a simulation of future air quality without additional controls or whether a simulation of candidate control strategies is to be conducted, one must first project the corresponding level of emissions resulting from growth, controls, or both. In the former instance, the projected emission inventory is called a baseline projection while in the latter it is called a strategy projection. Normally one baseline projection is performed for each projection year, usually 1987, and a later year (1995 for example). However, some urban areas may want to examine the effects of alternative levels of economic and population growth. In such cases, multiple baseline projection scenarios may be needed.

Several strategy projections will also need to be performed for each projection year.* These projections reflect varying combinations of individual control measures, such as RACT (reasonably available control technology), LAER (lowest achievable emission rate), I/M (inspection and maintenance), TCM's (transportation control measures), and possibly others. The strategy projections also reflect which sources would be controlled and when the controls would come into effect. If only final strategy projections are to be performed, having been formulated through use of the Airshed Model in a "sensitivity" mode, only one or two projections may need to be made. On the other hand, if a final control strategy is formulated by simulating specific candidate strategies, a considerable number of alternate strategy projections will need to be made.

*It may also be desirable to examine a candidate strategy in the base year.

As discussed in Chapter IV, Preparation of Model Input Data, the EMISSIONS and PTSOURCE files contain hourly emissions of eight pollutants. Furthermore, these emissions are in gridded form on the EMISSIONS file, there being no distinction between one source and the next. Obviously, neither baseline nor strategy projections can be performed at this level. As discussed in Chapter III, Data Needs, stationary source projections are made on an annual basis by source category. Mobile source projections are made for the entire transportation network down to the link level in terms of average daily traffic and peak hour traffic. The emissions, whether stationary or mobile, are recalculated and are disaggregated temporally. Hydrocarbons and nitrogen oxides are apportioned to the five carbon bond categories and to nitric oxide or nitrogen dioxide, respectively. Finally, the mobile source, point source, and area source emissions are assigned or allocated to the appropriate grid squares. Essentially then, performing a projection of emissions for a future year is equivalent to regenerating the hourly gridded inventory for model input.

B. FUTURE YEAR MODEL SIMULATIONS

Once the Airshed Model has been verified using one or more days of aerometric data and once the baseline emission projections have been performed, one is ready to simulate future ozone levels. Preferably more than a single day has been verified. If so, simulation of future year baseline emissions and subsequent formulation of control strategies should usually be based on the day having the highest ozone concentration. However, if the highest day occurred not as a result of urban generated ozone but rather as a result of transport, one will also want to formulate and evaluate control strategies on a day for which urban generated ozone predominates.

In addition to the projected emissions data, the starting points for assembling model inputs for future year simulations are the air quality and meteorological data files for the day or days selected for control strategy analysis. All modifications made to these files during the course of the verification analysis should be reflected in the input files used for future year simulations. The meteorological files, namely WIND, DIFFBREAK, REGIONTOP, TEMPERATUR, METSCALARS, and TERRAIN, are used directly and are not further modified in any way. In contrast, the air quality files, namely AIRQUALITY, BOUNDARY, and TOPCONC, must be adjusted to correspond to anticipated future year conditions, as discussed below.

1. Baseline Simulations

Simulating baseline conditions in a future year corresponds to a scenario in which growth occurs but no controls other than those having previously been adopted are considered. Data preparation programs are run using the projected baseline emissions to create the EMISSIONS and PTSOURCE files for model input. (These files were described previously in Chapter IV, Preparation of Model Input Data). The files containing air quality data may or may not require adjustment. Under a baseline scenario, sources outside the urban area may have no controls beyond those in place during the base year. In this case, an assumption could be made that transport at the upwind edge of the modeling region and aloft remains the same as in the base year, thereby requiring no adjustments to the BOUNDARY or TOPCONC files.

The AIRQUALITY file generally should be adjusted, however. This file contains the initial ambient concentrations for each pollutant at the beginning of the simulation. Initial conditions could be assumed to be proportional to the urban regional emissions. Future year initial conditions of hydrocarbons could then be approximated by taking the ratio of the regional future year hydrocarbon emissions to the regional base year emissions and applying this factor to the initial conditions for all five carbon-bond categories. However, natural background levels should be subtracted out first so that only the anthropogenic portions of the initial conditions are adjusted. In addition, if any pronounced temporal variation exists in the emissions ratio, this should be taken into account. Nitric oxide and carbon monoxide initial conditions could be approximated similarly using NO_x and CO emissions, respectively. Unfortunately, there is no such direct method for estimating future ozone and nitrogen dioxide initial conditions or those of other secondary photochemical pollutant species (PAN and BZA). Since the accumulation of these pollutants in the atmosphere is generally limited by the amount of reactive hydrocarbons emitted, use of a future year to base year hydrocarbon emission ratio could serve as a surrogate factor.

Model results may be presented as a printed map of ozone concentrations as shown in Figure VI-1 or as ozone isopleths as shown in Figure VI-2. The Airshed Model itself produces printed maps only; one number is plotted for each grid cell. Maps may be generated for a selected hour at any vertical grid cell level, but normally only ground-level concentrations are of interest when evaluating the need for controls. Computer plotting routines external to the model are required in order to display ozone isopleths.

2. Control Strategy Simulations

As indicated earlier, two different approaches to control strategy development may be taken. One is to use the Airshed Model in a "sensitivity" mode. Across the board reductions in hydrocarbon and/or nitrogen oxide emissions are made to varying levels. The principal advantage of this method is that it is relatively easy to do. The principal disadvantage is that it ignores the capability of the model to evaluate the effect of significant changes in the

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POLLUTANT: O3     DAY: 159  HOUR: 14-15

             AVERAGE AMBIENT CONCENTRATIONS (PPB) OF OZONE

     ----2---3---4---5---6---7---8---9--10--11--12--13--14--15--16---
     *                                                                *
  21 * 194 186 178 159 136 125 130 135 136 140 141 139 137 138 144   * 21
     *                                                                *
  20 * 214 204 199 186 165 145 143 149 143 140 140 139 138 136 133   * 20
     *                                                                *
  19 * 233 220 217 208 194 173 158 153 141 137 139 139 138 136 134   * 19
     *                                                                *
  18 * 242 228 226 220 210 195 175 156 144 137 137 138 137 136 134   * 18
     *                                                                *
  17 * 241 226 225 220 211 193 172 155 146 140 137 138 137 136 133   * 17
     *                                                                *
  16 * 229 214 212 207 199 178 160 148 143 140 138 137 137 136 133   * 16
     *                                                                *
  15 * 209 194 194 191 178 162 148 140 140 139 138 137 136 135 133   * 15
     *                                                                *
  14 * 185 171 171 170 160 147 137 134 136 137 138 137 136 135 133   * 14
     *                                                                *
  13 * 160 145 144 145 144 135 128 123 128 135 137 137 136 135 133   * 13
     *                                                                *
  12 * 140 122 121 123 130 128 121 117 121 134 135 136 136 135 133   * 12
     *                                                                *
  11 * 136 110 106 110 118 122 117 113 119 130 134 136 136 135 133   * 11
     *                                                                *
  10 * 134 111 106 106 112 119 125 126 126 129 132 134 135 135 133   * 10
     *                                                                *
   9 * 133 113 107 104 107 113 118 122 127 128 130 133 134 134 133   *  9
     *                                                                *
   8 * 135 117 113 107 107 111 119 126 126 127 128 130 133 134 133   *  8
     *                                                                *
   7 * 135 119 117 111 107 113 120 124 126 125 124 125 129 132 132   *  7
     *                                                                *
   6 * 135 121 121 116 108 111 121 122 121 121 121 123 126 129 130   *  6
     *                                                                *
   5 * 136 122 124 123 116 113 123 124 123 123 123 123 125 127 129   *  5
     *                                                                *
   4 * 136 124 126 126 125 126 125 125 125 125 125 125 125 127 129   *  4
     *                                                                *
   3 * 136 125 126 126 123 127 127 126 126 126 126 126 126 127 129   *  3
     *                                                                *
   2 * 135 126 127 127 127 128 128 128 128 128 128 128 128 129 129   *  2
     *----------------------------------------------------------------*
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FIGURE VI-3, EXAMPLE OF PRINTED MAP OUTPUT FROM AIRSHED SIMULATION.

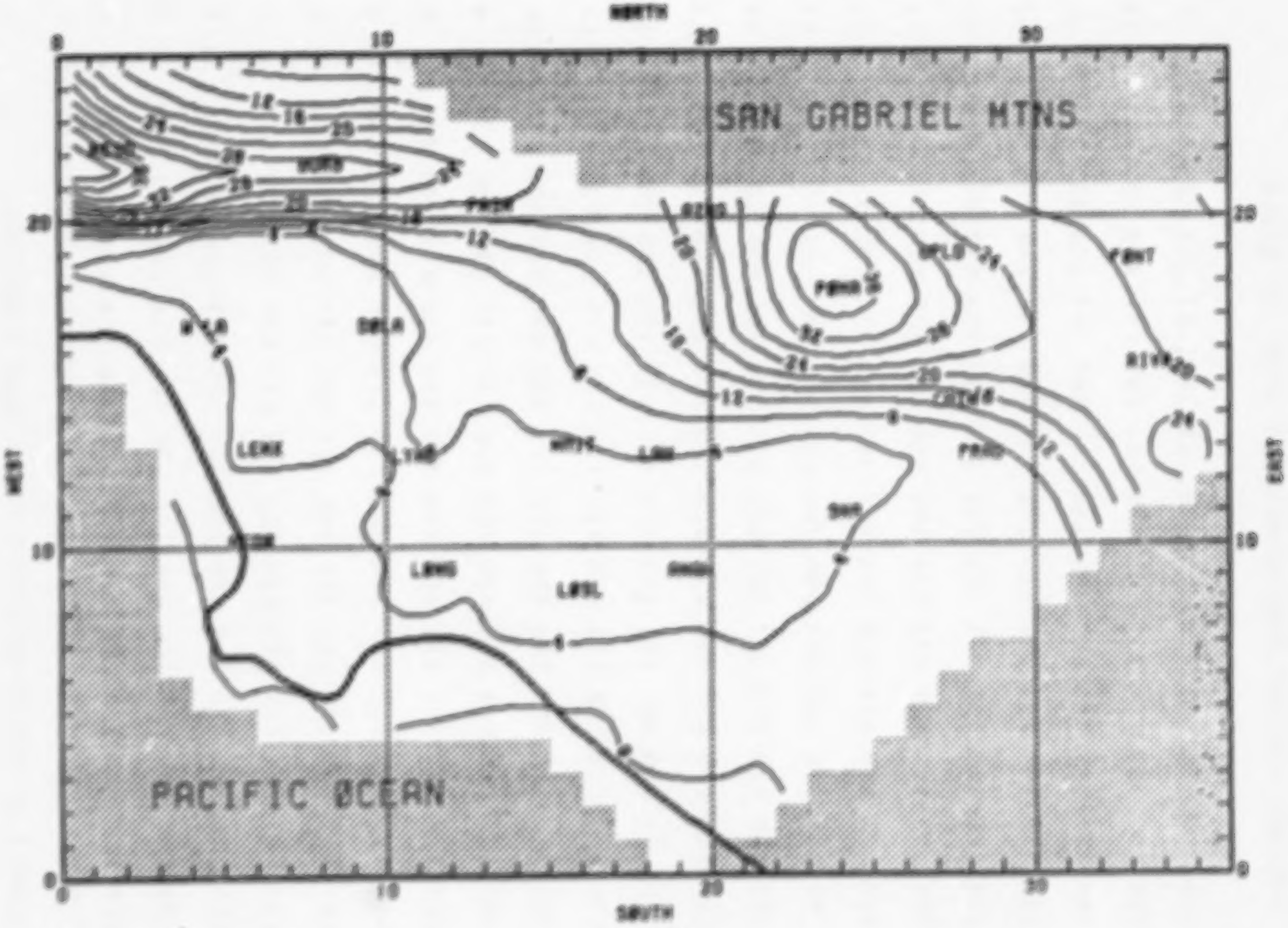

NORTH
SOUTH
WEST
EAST
SAN GABRIEL MTNS
PACIFIC ØCEAN
DØLA
LENX
LØNG
LØSL
FØNT
RIVR
PØMA
0
10
20
30

FIGURE VI-2. EXAMPLE OF A PLOTTED CONTOUR MAP OF GROUND-LEVEL OZONE CONCENTRATION ESTIMATES. (Tesche and Burton, 1978).

locations of emission sources and in the reactivity of the emissions. The final strategy selected on this basis may either be more stringent than necessary or less stringent depending on the manner in which the overall emission reduction is actually distributed among sources, whether elevated or ground-level, more or less reactive, upwind or downwind. The preferred method is to project the effects of different combinations of control measures on future year emissions, on a source by source basis as described above in Section A, Preparation of Future Year Emissions. This method allows one to use the Airshed Model to its full potential.

Whichever approach is taken, it is helpful to have some notion beforehand of the approximate level to which total regional hydrocarbon emissions must be limited in order to meet the ozone standard. The Empirical Kinetic Modeling Approach (EKMA) offers a simple technique (EPA, 1977c). Using the EKMA standard curves, which show the relationship between ambient levels of hydrocarbons and nitrogen oxides and the level of ozone under a set of standard conditions, one may estimate an approximate percent hydrocarbon reduction needed to reach the ozone standard. Two pieces of information are required: the ozone "design value" and the $NMHC/NO_x$ ratio. The design value, as described in "Guideline for the Interpretation of Ozone Air Quality Standards" (EPA, 1979), is the ozone concentration which has an expected exceedance of once per year. The design value is determined statistically irrespective of the particular day selected for control strategy analysis. However, the $NMHC/NO_x$ ratio should correspond to the mean of the urban (as opposed to the upwind or downwind) air quality monitoring sites for the 6 to 9 a.m. period on the day or days selected for control strategy analysis. Once an approximate percent hydrocarbon emission reduction for the base year is estimated using the EKMA curves, this may be translated into a percent reduction for any particular baseline projection year. This is done by first computing the reduced base year regional hydrocarbon emission total and dividing by the projection year baseline emission total. This of course is subtracted from 1.00 and then multiplied by 100 to obtain the percentage reduction. This provides a first estimate of the overall level of control that may be needed. With this information one can begin to identify the control measures that may be necessary and to formulate candidate control strategies.

Boundary conditions for the modeling region are important regardless of the approach taken. Equity requires that a downwind city should not have to exercise additional controls merely because an upwind city fails to meet its responsibilities to attain the ozone standard. Therefore, the air quality planner will want to assume the upwind city is meeting the standard. How then can the boundary conditions be made to reflect this? An ideal approach would be to use a regional photochemical model. A regional model is now under development by the Environmental Sciences Research Laboratory, U. S. Environmental Protection Agency, Research Triangle Park, North Carolina, but is not yet available. A simple technique is to assume that the change in ozone transport aloft and along the upwind edge of the modeling region is proportional to the change in ozone levels in the upwind city. Stated another way, the ratio of the upwind city "design value" for ozone during the base year to the ozone standard is the same as the ratio of the ozone boundary value in the base year to the boundary value in a future year. If the maximum ozone level for the upwind city is known for the specific day being modeled, that value should be used in place of the design value. Transported precursors (hydrocarbons and nitrogen oxides) should probably not be reduced unless it can be demonstrated the upwind city is the source of the emissions. Generally, the relatively low levels of transported precursors normally observed are thought to have their origin in nonurban areas immediately upwind of a metropolitan area. Once an overall reduction in transported ozone has been estimated, the BOUNDARY and TOPCONC files must be recreated to reflect the change.

If the sensitivity approach is used to develop control strategies, the emission reductions selected should generally correspond in an overall sense to specific control measures. For example, preliminary analyses may indicate hydrocarbon reductions in the 25 to 50 percent range, relative to future year baseline emissions are needed. Rough estimates of the effect of "RACT" on point sources might show that a 22 percent reduction in total regional hydrocarbons could be achieved while "LAER" might provide another five percent. Application of a strong "I&M" program might reduce regional emissions by four percent and a combination of "TCMs" another two percent. In this example, one might select overall reductions of 22 percent (RACT) 33 percent (LAER/I&M/TCMs) and 50 percent. The gap between 30 and 50 might, for instance, be ascribed to new source review incorporating a stringent offset policy.

Across-the-board emission reductions such as these are readily accomplished through the use of techniques provided in the data preparation programs. The EMISSION FACTORS packet is suitable for this purpose. Initial concentrations contained on the AIRQUALITY file should also be reduced by the same factor as the emission rates. This is done by adjusting the station readings used as input to the data preparation program; the program is then reexecuted to create a new AIRQUALITY file.

Assuming the Airshed Model simulation runs show that the ozone standard is met and exceeded (i.e., "bracketed") within the range of hydrocarbon reductions selected, one may interpolate between runs to estimate the overall percent reduction required to just reach the standard. It is then necessary for the air quality planner to select what combination of control measures applied to which sources with what level of control are needed to attain the standard. Alternate sets of measures should be tentatively selected because the key step in the sensitivity approach is confirming one of these strategies by means of actual Airshed Model simulations. This is done by performing detailed emission projections (as described above in Section A. Preparation of Future Year Emissions) followed by running of the Airshed Model. The model should be run for each of the high ozone days previously verified. Hopefully, one of the strategies chosen will show attainment on all test days. If not, more stringent measures are needed and the process is repeated.

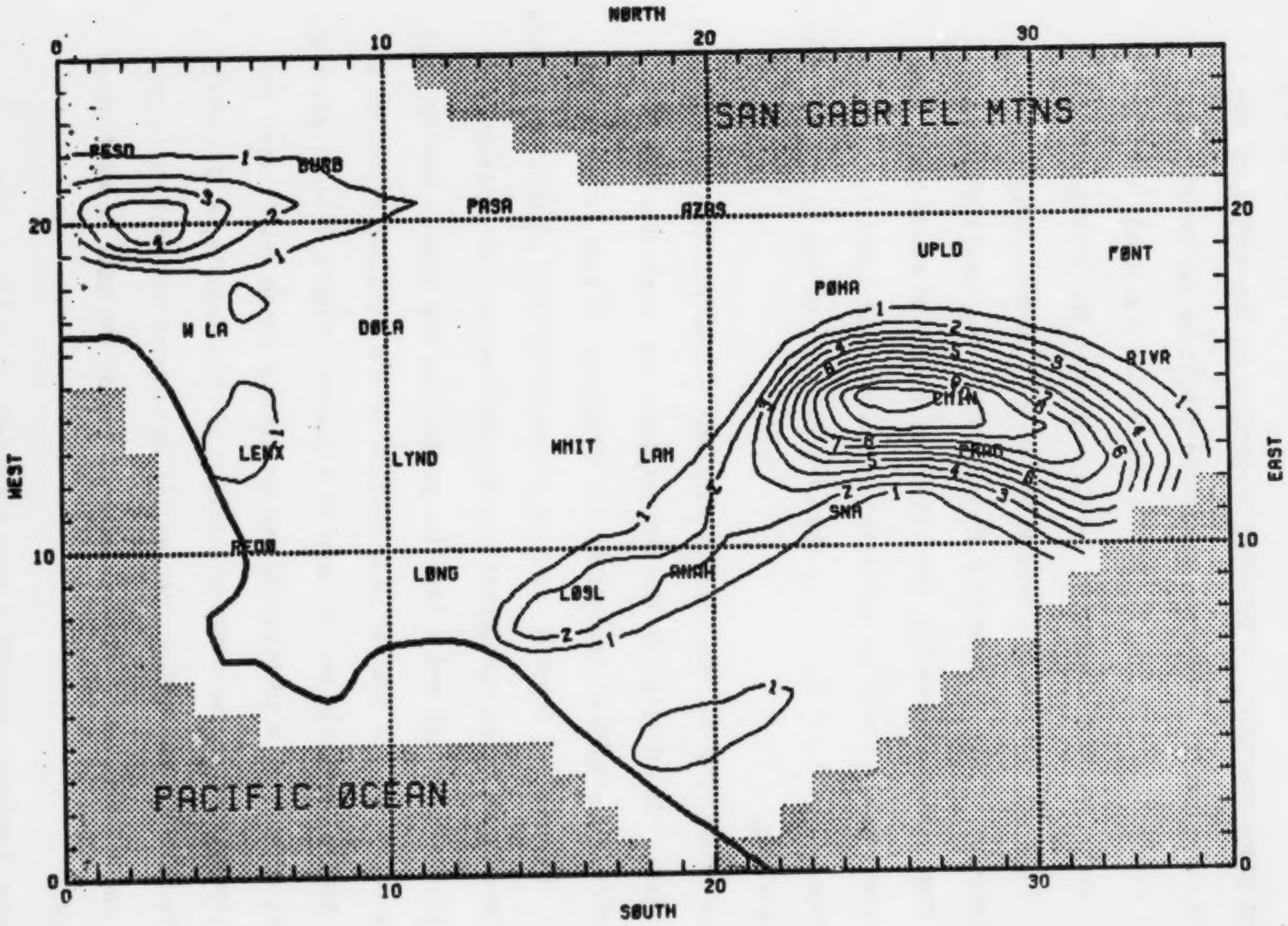
The alternate and preferred approach differs primarily in the manner by which control strategies are formulated. Rather than making area-wide emission reductions, one performs detailed projections of candidate strategies composed of various control measures individually or in combination. Combining them in different proportions to different source types, one may arrive at any number of candidate strategies. For example, "RACT" reductions might be applied to refineries and surface coating operations but not to service stations in one strategy while another strategy might specify "LAER" reductions for all three. These candidate strategies are then simulated using the Airshed Model. The results are then evaluated in the context of the strategy's potential for attaining the ozone standard.

Once the candidate strategies have been simulated and the results analyzed, the air quality planner is in a good position to select those control measures and the source types to which each should apply which in combination will attain the standard. If the candidate strategies have been carefully selected in relationship to one another, a final strategy may be arrived at readily with a minimum of trial and error while assuring, when tested, attainment will indeed be shown.

Regardless of the approach taken, once a "final" strategy has been selected, it should be tested to confirm that it will provide for attainment of the ozone standard. A detailed projection of the effect of the strategy on emissions as previously described should be performed. Airshed Model simulations are then conducted on several previously verified high ozone days, not just the one or two days adopted for strategy formulation, in order to test the strategy under several meteorological and air quality scenarios. This is important because differing levels of ozone transport from upwind urban areas and differing levels of ozone carry over from a previous day, as well as differing meteorological conditions during the days modeled, will all influence the effectiveness of the particular control strategy selected.

Airshed Model results from control strategy simulations may be presented in various ways. In addition to the printed maps and isopleth plots mentioned previously, graphical techniques for comparing strategies directly are useful. Figure VI-3 shows a "deficit enhancement" plot on which isopleths of the difference in ozone concentrations between two control strategies or between a control strategy and a baseline projection are shown. Having such a plot, the magnitude and spatial distribution of the relative effect of a particular control strategy may be seen at a glance. Figure VI-4 illustrates the temporal effects of a sensitivity run on maximum ozone levels over the course of simulations on two different days. In this example, a 30 percent reduction in both NO_x and hydrocarbon emissions reduced the peak ozone concentration about 15 percent. However, the timing of the peak concentration is unchanged.

The ozone isopleths resulting from different control strategies may be analyzed further by determining at hourly intervals the area over which


NØRTH
SØUTH
WEST
EAST
0
10
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SAN GABRIEL MTNS
PACIFIC ØCEAN
RESD
BURB
PASA
AZBS
UPLD
FØNT
PØMA
RIVR
W LA
DØEA
CHIN
PRAD
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FIGURE VI-3. DEFICIT ENHANCEMENT PLOT ILLUSTRATING THE PREDICTED EFFECT OF A CONTROL STRATEGY (Tesche and Burton, 1978).

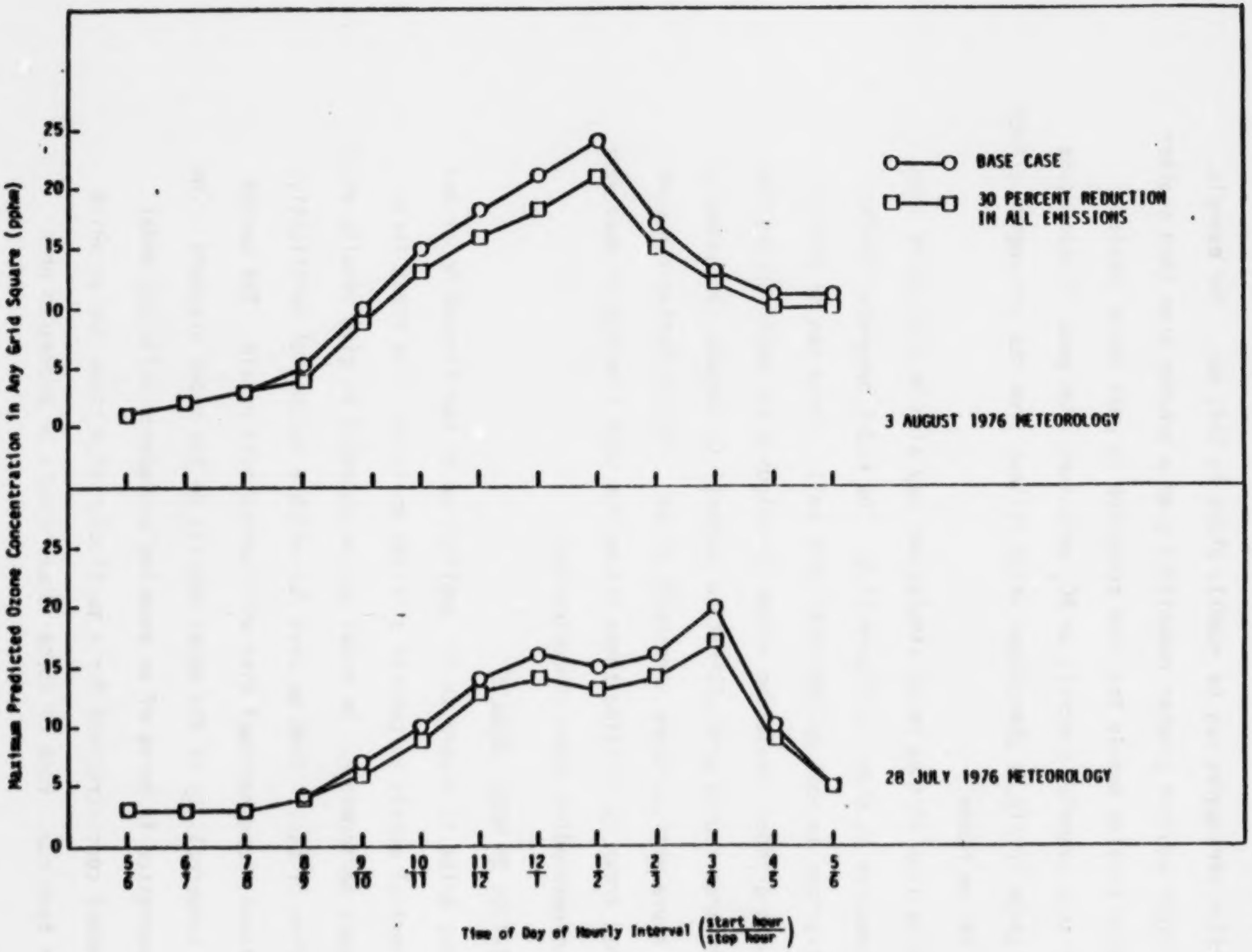

FIGURE VI-4. TEMPORAL EFFECTIVENESS OF A SENSITIVITY RUN ON PEAK OZONE CONCENTRATIONS (Anderson, et al., 1977).

estimated ozone levels exceed various threshold values. The results may then be summarized graphically as shown in Figure VI-5. Differences between two otherwise similar strategies may be readily shown in this way. For example, one strategy might achieve greater reductions over a greater area than another even though both provide nearly the same reduction in peak ozone levels. (Note that in this example, controls on NO_x emissions from power plants cause higher urban ozone levels, a phenomenon which follows from the scavenging effect nitric oxide has on ozone.)

The results from Airshed Model simulations may also be translated into population exposures as shown on Figure VI-6. The model generates hourly ozone concentrations in each ground-level grid cell. These can be used in conjunction with gridded population values (previously estimated during the development of area source grid allocation factors) to compute the number of person-hours above various ozone threshold values. The population exposure curves are then drawn by plotting these values for each strategy or each year against the corresponding ozone concentration.

C. INTERPRETATION OF MODEL RESULTS

Two issues arise in regard to the application of the Airshed Model and other photochemical models to control strategy analysis. The first issue relates to model performance. No model can be expected to give results which are totally free of bias. Even on days for which a successful verification has been achieved, some residual bias will undoubtedly remain. The second issue is the comparability of the model results to the ozone standard. The standard is expressed in terms of an expected exceedance while the model results represent concentrations for a particular high ozone day on which the model has been run. Both of these issues should be addressed when

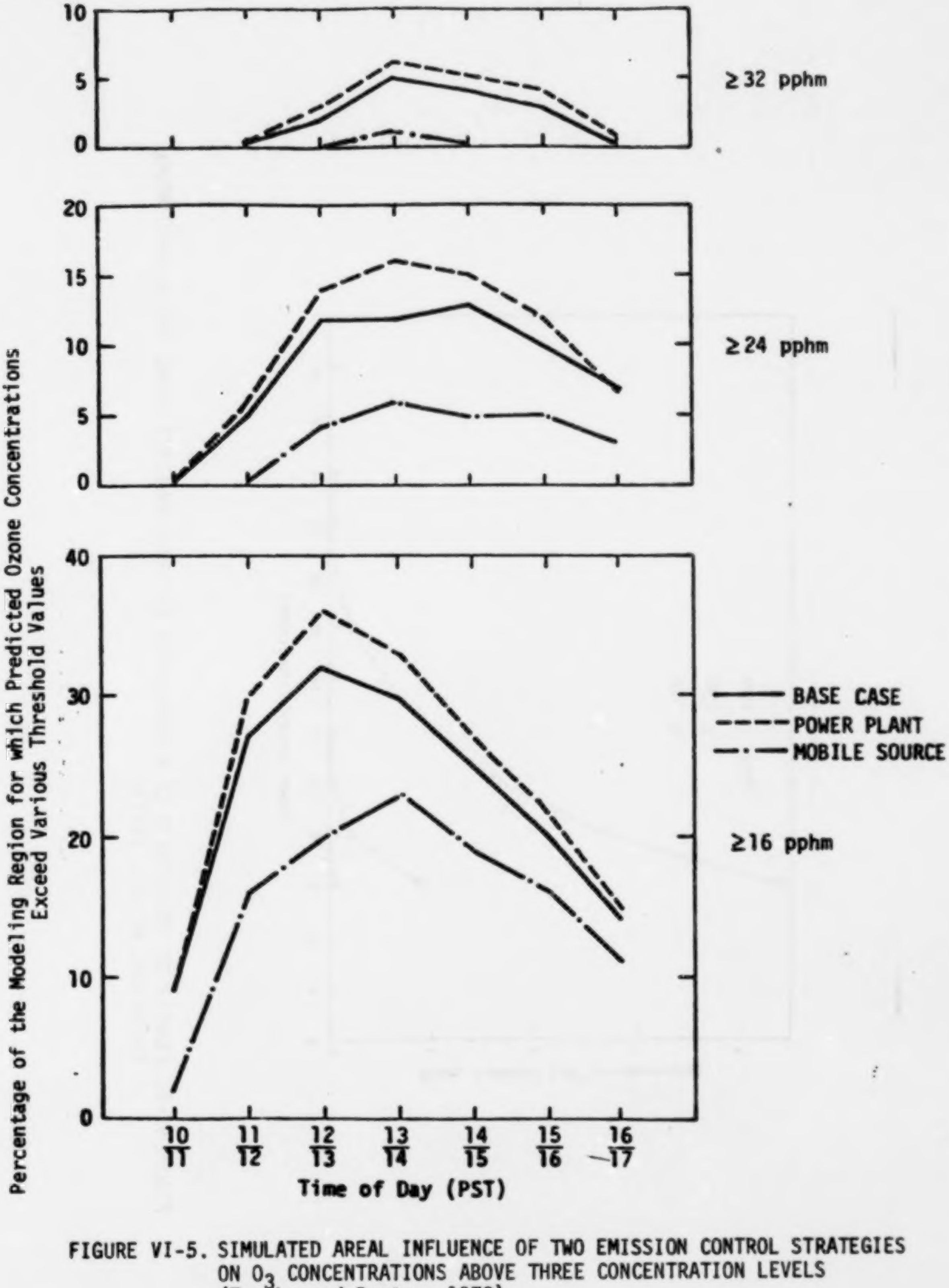

FIGURE VI-5. SIMULATED AREAL INFLUENCE OF TWO EMISSION CONTROL STRATEGIES ON O_3 CONCENTRATIONS ABOVE THREE CONCENTRATION LEVELS (Tesche and Burton, 1978).

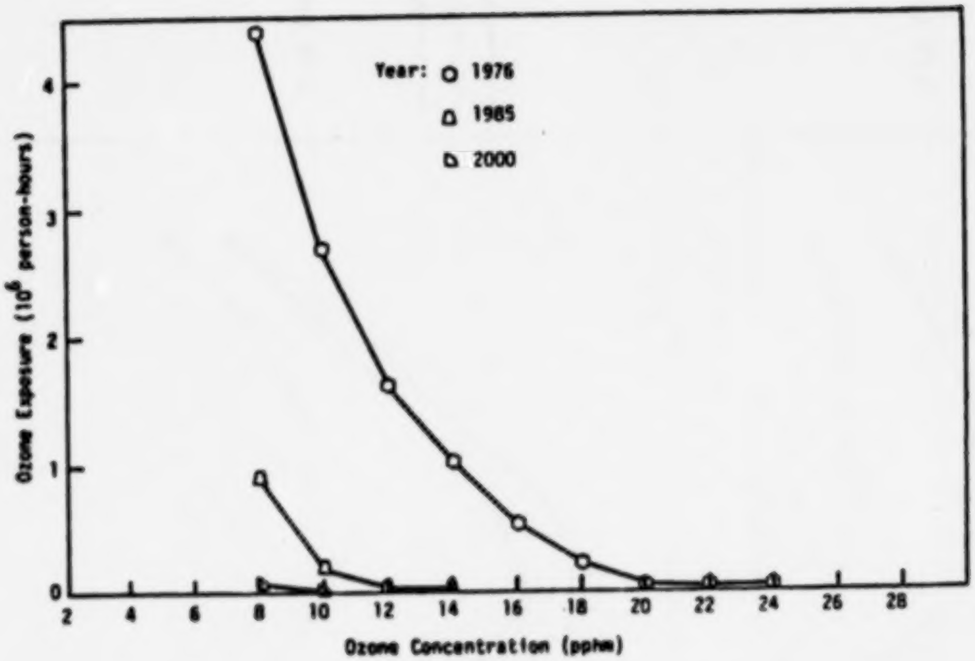

FIGURE VI-6. EXAMPLE OF THE RESULTS OF A POPULATION EXPOSURE ANALYSIS USING THE AIRSHED MODEL (Anderson, et al., 1977).

applying the model to control strategy analysis to avoid either overstating or understating the level of control required to meet the ozone standard.

The best way to eliminate model bias is to adjust the model itself to remove the bias at its source. However, such "fine tuning" of the model could be quite time consuming and may be impractical under the time and resource constraints imposed upon the modeling effort. Calibration offers an alternative to reformulating the model. Calibration attempts to adjust the model ozone estimates themselves to better correspond with ozone observations. Calibration does not necessarily improve the accuracy of the model; rather it simply ttries to compensate for any bias present in the results. Calibration is not a substitute for good model performance.

The second model interpretation issue arises when the prototype day has a different maximum ozone concentration that does the design day. The prototype day is the particular day on which the model is run. The design day is a hypothetical day on which the ozone design value occurs. The design value is the ozone concentration which has an expected exceedance of once per year. Methods for determining the design value are discussed in "Guideline for the Interpretation of Ozone Air Quality Standards" (EPA, 1979).

There are no assurances that a day with an ozone concentration equal to the design value will occur during the three-month aerometric data collection study. Typically, the day or days selected for modeling will have a maximum observed ozone concentration less than the design value. Therefore, the ability to demonstrate on a prototype day that the ozone standard is not exceeded under a given emission control strategy does not necessarily assure that the ozone standard will not be exceeded on the design day. The only entirely satisfactory way to address the design day issue is to actually evaluate a given strategy using the Airshed Model on the design day. However, given that the prototype day does not correspond to the design day, an objective technique is needed to relate model estimates on the prototype day to the design day. The question becomes, how can the model estimates be adjusted so they can be used for comparison with the ozone standard? An attempt at answering this question has been made by the Association of Bay Area Governments (ABAG, 1979).

CHAPTER VII. RESOURCE REQUIREMENTS FOR AN AIRSHED MODEL STUDY

Use of the Airshed Model in an urban area for control strategy planning is an expensive undertaking. As described in earlier chapters, a large data base needs to be amassed first. Emissions data must be collected, compiled, reviewed, and analyzed. Field studies to gather the necessary meteorological and air quality data must be planned and executed. The resulting data must be compiled, reviewed, validated, and analyzed. Each of these two data collection activities involve long lead times and are generally done largely under contract. Modeling itself requires specialized skills and experience not commonly found in local pollution control agencies and is therefore normally a contract activity. Modeling verification may be a lengthy process but one which must be accomplished before control strategy evaluation and testing can begin. Execution of the Airshed Model requires the use of a large high speed computing facility. Running times are long and computer costs are substantial.

A. MODELING PERSONNEL

While the number of persons needed to perform the modeling verification and control strategy analysis phases of the overall study is not necessarily large, a diversity of knowledge and experience is required. The various disciplines needed include:

- engineering
- computer science
- meteorology
- chemistry
- statistics

Because personnel normally follow disciplinary lines, the modeling team should include at a minimum an air pollution engineer, a systems analyst or programmer, an air pollution meteorologist, an atmospheric chemist, and a statistician. The engineer and computer specialist are often involved in most aspects of the modeling. The extent of involvement of the meteorologist, chemist, and statistician depends on their individual background and experience in modeling. Their abilities are essential in certain key phases of the study, yet their special expertise is not necessarily required throughout the entire study. For example, the skills of the meteorologist, chemist, and statistician are not normally needed during the control strategy evaluation phase. However, any one of the team participants, regardless of their particular disciplines, may take on the lead role in the study depending on his or her experience in photochemical modeling.

The air pollution engineer should have experience in applying models and should be familiar with emission inventory practices and techniques. During the control strategy evaluation phase, he has primary responsibility for preparing strategy emission projections, for preparing the model input data, and for evaluating the model results. During the model verification phase, he is involved in evaluating verification problems and conducting sensitivity analyses, particularly as related to emissions data.

The air pollution meteorologist should have a background in boundary layer meteorology and modeling. It is his responsibility to prepare the meteorological data for model input. This includes specifying the wind field, mixing heights, and stability data for the modeling region. He is heavily involved in the verification phase in evaluating the effect of meteorological variables on model performance. An in-depth analysis of the meteorological data base and the use of several data preparation schemes may be needed before satisfactory results are achieved.

The atmospheric chemist should have a background in ambient monitoring and the chemistry of ozone formation. He should be especially familiar with the carbon-bond mechanism and how it treats various organic compounds. The atmospheric chemist is responsible generally for assisting in the assessment of the reasonableness of the emission inventory and specifically for reviewing how the organic emissions from various source types have been assigned to the five carbon-bond categories. He is also responsible for preparing the ambient nonmethane hydrocarbon data. The chemist plays a key role in evaluating air quality data aloft and upwind in order to prepare model boundary conditions. He also assists in the preparation of initial conditions. The atmospheric chemist joins in the verification effort to determine whether the air quality data is in need of re-examination and whether the model chemical kinetics are performing properly.

The computer specialist is the backbone of the modeling team. It is his job to carry out many of the data manipulations necessary to create the files requested by the other project team members. Frequently, this may involve modifications to the existing data preparation programs or entire new programs may need to be written. Most of the data manipulations necessary for performing strategy emission projections, followed by the necessary splitting, gridding, and recombining, must be done using computer processing. Obviously, the computer specialist must be thoroughly familiar with the computer system on which the model is to be exercised. He must be knowledgeable concerning system design, data storage, tape handling procedures, and structured programming. The computer specialist must, of course, know how to operate the large Airshed Model system of programs and files. Finally, he should have a working knowledge of computer plotting software so that model outputs (and inputs) can be examined and evaluated graphically.

The statistician is primarily involved in evaluating model performance. It is he who is responsible for identifying the performance measures to be used, for applying, and for interpreting such measures. He assists in examining the model results to isolate probable causes of verification problems. The statistician works with the computer specialist in manipulating the data, either numerically or graphically. He may also be called upon at the beginning of the modeling study to assist in examining and analyzing the data base, particularly the aerometric data.

B. COMPUTER FACILITY

The Airshed Model computer program is written entirely in FORTRAN. The executable module requires 61K 36-BIT words of memory for operation on a UNIVAC 1144. On the same computer, running time for the model is approximately 15 minutes per hour of simulation for a modeling region of 300 grid squares and four vertical layers, i.e., 1200 grid cells altogether. Since running time depends primarily on the size of the modeling region, more grid cells would require proportionally more time. However, this time can also vary somewhat due to the shorter time steps necessary for increasing wind speeds. If the user-defined modeling region is too large to fit into the available core of the host computer, a segmentation process is available which divides the region into one or more rectangular segments. Using segmentation, the data arrays for all segments are maintained in secondary storage while the arrays for the segment being processed reside in core.

The times and core requirements given above reflect a modeling region divided into two segments.

Initially the model requires the operation of eleven preprocessor programs. Each of these programs performs a similar function in that each prepares and formats the various types of data required for input to the model. Each program requires approximately 60K 36-BIT words of memory for operation on a UNIVAC 1144. Also, each program requires an average of approximately two minutes of running time. The files produced by these programs can be written on either magnetic tape or disc. Eleven output files are produced for input to the model. In addition to these eleven, the segmented modeling region described above requires the use of seventeen external mass-storage files requiring an overall total of approximately 725,000 36-BIT words.

C. PROJECT TIMETABLE

A project the size of a photochemical modeling study using the Airshed Model poses considerable uncertainty not only in regard to its cost, but also in regard to the time required for its completion. Figure VII-1 represents the kind of study timetable one may expect. Overall, a study using the Airshed Model may be expected to take three years or more.

Once the local pollution control agency has made the decision to perform an Airshed modeling study, initial planning begins. This may take about six months. An analysis of the existing emissions data base and the historical meteorological and air quality data must be carried out. With this information, decisions can be made on the dimensions of the modeling region and on the exact data needs for the study. The adequacy of the existing monitoring network and the need for additional meteorological and air quality monitoring sites and instrumentation must be assessed. The

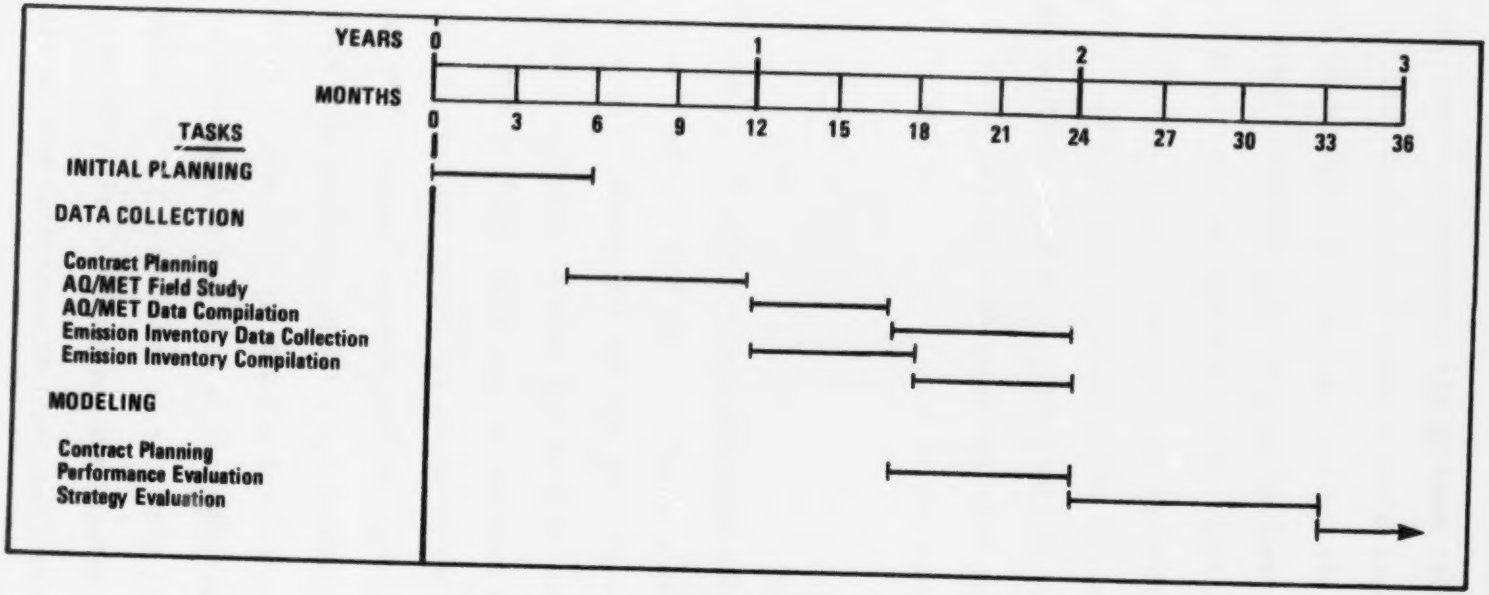

Figure VII-1. A Photochemical Modeling Study timetable.

requirements for upper air meteorological and air quality data must be established. The extent to which the existing stationary source emission inventory meets the needs of the study must be assessed and additional data needs must be identified. The level of effort required to take the existing transportation data base and use it for generating the mobile source emission inventory must be estimated. The assistance of a contractor familiar with the Airshed Model and its requirements is a valuable part of the initial planning effort. Toward the end of the initial planning phase, it should be possible to make reasonable estimates of the resources required to perform the study.

Soon after the initial planning, the local agency will want to decide on the extent of contractor involvement. This depends on the in-house man-hours available to devote to the project and the availability of outside funding. Contractors are oftentimes heavily involved in the data collection effort. Depending on agency contracting procedures, contract solicitation, selection, and award can require seven months of elapsed time, if all goes well.

Once one or more contractors have been selected to operate supplementary surface monitoring sites, collect aircraft and upper air meteorological data, and analyze hydrocarbon grab samples, the field study can begin. For a three month data-collection period, one should probably count on at least two months of preparation time. New monitoring stations and associated instrumentation must be acquired, installed, and readied. Aircraft must be equipped, the flight crew assembled, and flight plans drawn up. Radiosondes, pibals, and associated tracking equipment must be obtained and release sites prepared. Existing surface monitoring stations may need to be reequipped or overhauled. With the onset of the "oxidant season," data collection begins. After it is collected, the data must be validated, archived, reviewed, and analyzed. Before the data is ready for modeling, another seven months will likely have passed.

Concurrent with the aerometric data collection effort is the emissions data collection effort. Agency stationary source files must be reviewed and updated as necessary. Area source emissions must be determined for each county in the modeling region and allocation factors must be developed to allocate them to the grid system. Temporal profiles must be developed for each source as do profiles for apportioning hydrocarbon and nitrogen oxide emissions to the five carbon-bond categories and to NO and NO_2. Diurnal traffic distribution data must be developed, VMT estimates made, and speeds computed for the transportation inventory. Vehicle operating characteristics must be estimated. Approximately six months may be required for collecting these various data. Another six months may be needed to ready network emissions models, to prepare other computer software, and then to generate the hourly gridded emission inventories for model input.

Well before the emissions and aerometric data bases are expected to be ready for modeling, the agency should obtain the services of a modeling contractor. As for the data collection effort, seven months may be required to consummate a contract.

Model performance evaluation begins with an analysis of the data base. The meteorological and air quality data must then be prepared for model input. Once the model is run, the results must be evaluated and any problems corrected. This requires about nine months. The formulation of candidate control strategies and the selection and testing of a final strategy are open-ended activities which may last as long or longer than the model performance evaluation.

D. OVERALL PROJECT COSTS

Table VII-1 shows a range of overall project costs, exclusive of computer costs, broken down by major activities. All cost items are assumed to be

Table VII-1. Photochemical Modeling Study Costs

Activity	Cost[1] Low	($1000)	Cost[1] High	Computer Time[2] Low	(Hours)	Computer Time[2] High
PLANNING	20		40	-		-
DATA COLLECTION						
Surface AQ/MET Data	250		550	1		3
Upper Air MET Data	30		100	1		1
Aircraft AQ Data	-		150	-		1
Organic Species AQ Data	20		40	-		-
Emissions Data	150		850	15		30
Subtotal	450		1690	17		35
MODELING						
Performance Evaluation	100		180	7		12
Strategy Evaluation	80		110	8		16
Subtotal	180		290	15		28
TOTAL	650		2020	32		63

[1] Contract costs, excluding computer costs, 1979 dollars.

[2] For a CDC 7600 machine.

done outside the local agencies, under contract. Costs for managing the project, which may require one or two man-years in and of itself, are assumed to be absorbed by the agency's own manpower resources and not require external funding. Any tasks performed by the agency in-house will reduce project costs proportionally. Also shown in Table VII-1 are approximate computer time requirements for a machine such as the CDC 7600. Based on these estimates, total noncomputer costs for a photochemical modeling study may range from a low of 600 thousand dollars to a high of 1.9 million. Between 75 and 85 percent of this is for data collection while the remainder is for modeling and for contractor assistance in the initial planning of the project. In addition, at a unit cost for computer time of two thousand dollars per hour on a machine such as the CDC 7600, total computer costs may range from 65 to 125 thousand dollars.

Previous experience in planning photochemical modeling and aerometric and emissions data collection studies shows that initial planning costs may range from 20 to 40 thousand dollars. This is the cost at the start of the project for contractor assistance in planning the overall study and of determining what the particular data needs are.

Collection of surface air quality and meteorological data is usually the largest single cost item in a photochemical modeling study. As indicated in Table VII-1, costs may vary from 250 to 550 thousand dollars or more. The cost depends on the number of new monitoring sites required and on any additional monitoring equipment needed at existing state and local agency sites. The cost figures shown here assume that all new sites are installed and operated under contract. No costs are included for operating existing monitors since these costs are already being incurred by state and local agencies. In Philadelphia, (PA-NJ-DL-AQCR) for example, where an Airshed Model application is underway, operation of five new sites for three months cost 250 thousand dollars. This includes data collection, compilation, validation, review, and analysis but does not include the cost of instruments, which were provided to the contractor. These five sites were supplemented by 17 state and local sites. Some computer time is also required to compile and analyze the entire surface aerometric data base.

Other cities where photochemical modeling studies are being planned are New York, Boston, Baltimore, and Washington, D.C. Estimated costs for surface aerometric data range from 550 thousand dollars in New York to 350 thousand in Baltimore. In Baltimore, four new sites are proposed to supplement seven existing sites which are being upgraded while in New York (NY-NJ-CN AQCR) the number of new and existing sites are 10 and 20 respectively.

Upper air meteorological data consists of rawinsonde, pibal, and acoustic sounder measurements. Among cities now being studied, cost estimates range from 30 to 100 thousand dollars. Equipment and operating costs are included. The high estimate of 100 thousand dollars is for Boston where no sites now exist and a radiosonde and two pibal sites are planned. At the low end, New York, a radiosonde site is available; two additional pibal sites are planned. In Philadelphia, 50 thousand dollars was expended for a single radiosonde site at which hourly pibal releases were also made.

Measurements of air quality data aloft using instrumented aircraft may or may not be taken as discussed in Chapter III. Data Needs. It has been estimated to cost 150 thousand dollars for 15 in-flight days. This also includes the cost of standby flight crews ready to fly during a typical three month summer study. However, these are only operating costs and do not reflect the cost of equipping an airplane with instruments.

A cost of 30 thousand dollars has been estimated for collecting 200 grab samples and conducting a complete organic species analysis using gas chromotography. The cost for a given study area depends on the number of samples analyzed.

The cost of developing an hourly gridded emissions inventory for model input is not so much dependent on city size, either in terms of geographic area or population, but rather on the condition of the existing data base. Contract costs may range from a low of 150 thousand dollars to a high of 850 thousand dollars for an inventory of mobile and stationary sources. In Baltimore, where the stationary source inventory is relatively complete and current, an estimated 70 thousand dollars is needed to derive the necessary spatial and temporal resolution, to develop VOC and NO_x pollutant profiles, and to perform two baseline projections. Another 95 thousand dollars is needed to generate the mobile source emission inventory, making the total inventory costs for Baltimore approximately 170 thousand dollars. In comparison, in the Metropolitan New York (NY-NJ-CN) AQCR, over half of an estimated 850 thousand dollar total cost is needed just to collect the data necessary to develop a basic annual inventory of point and area sources. Only 125 thousand of the total is needed for mobile sources. In the metropolitan Washington area, a total cost of 250 thousand is estimated of which 140 thousand is for mobile sources and 110 for stationary sources. These costs all include the cost of computer processing. In Baltimore, 28 thousand dollars has been budgeted for computer processing to generate mobile source emissions for model input from the transportation inventory. In Tulsa, 19 thousand dollars was expended for stationary source emissions computer processing.

In addition to the basic work of collecting and assembling the emissions data and manipulating it for model input, it is necessary to oversee closely the inventory effort and to thoroughly review the emissions data. This quality assurance function, if done under contract, may cost between 25 and 50 thousand dollars. However, these costs are not included in Table VII-1 where it has been assumed the local agency will perform this function without external funding.

The cost for model verification and control strategies depends on the number of Airshed Model runs and the size of the modeling region (and therefore the size of the data base). The same is true of the estimated computer time. Modeling costs range from 180 to 290 thousand dollars. Model verification includes the cost of analyzing the data and preparing it for model input as well as the simulations themselves, exclusive of computer costs. Also shown in Table VII-1 are estimated computer time requirements. At least two trial simulations are assumed necessary to achieve satisfactory model performance on any given day; however, more may be required. Model verification on three or four different days is also assumed. Control strategy analysis includes the cost of performing strategy emission projections and of running baseline simulations and candidate control strategy simulations. Anywhere from five to 15 runs may be required depending on what control measures are desired to be evaluated. In addition, final strategy confirmation runs on three or four days are also included. It should be realized that in running a model as large as the Airshed Model, a significant amount of computer time can be expended on wasted runs, runs for which no meaningful output results, due to various pitfalls and errors. The experience of one agency with a different model was that for every successful run, an average of 2.5 runs had to be made altogether (ABAG, 1979).

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APPENDIX

TECHNICAL DESCRIPTION OF THE AIRSHED MODEL

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TECHNICAL DESCRIPTION OF THE AIRSHED MODEL*

The development of the Airshed Model is described in numerous reports which detail the derivation of the model and the steps within each algorithm and subroutine. These reports were mentioned previously in the Foreword to this document. Although quite useful for developing an understanding of the model, their length makes their use difficult. This appendix provides a brief technical description of the model so that users can become familiar with the basic concepts and equations used in the model without having to peruse all the available detailed material. Since this appendix is not intended as a guide to the use of the model, none of the input or output functions of the model or data storage manipulations within the model are described.

A. THE BASIC EQUATION

The basis for the model is the continuity equation, which expresses the conservation of mass of each pollutant in a turbulent fluid in which chemical reactions occur. This equation can be written:

$$\underbrace{\frac{\partial c_i}{\partial t}}_{\text{Time Dependence}} + \underbrace{\frac{\partial (uc_i)}{\partial x} + \frac{\partial (vc_i)}{\partial y} + \frac{\partial (wc_i)}{\partial z}}_{\text{Advection}} = \underbrace{\frac{\partial}{\partial x}\left(K_H \frac{\partial c_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_H \frac{\partial c_i}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_V \frac{\partial c_i}{\partial z}\right)}_{\text{Turbulent Diffusion}}$$

$$+ \underbrace{R_i}_{\text{Chemical Reaction}} + \underbrace{S_i}_{\text{Emissions}} \quad , \tag{1}$$

where c_i represents the pollutant concentration and is a function of space (x,y,z) and time (t). This equation describing the dynamic behavior of reactive pollutants is fully three-dimensional. Further examination of the equation indicates that the following physical and chemical processes are considered in the Airshed Model:

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*Adapted from Reynolds, Tesche, and Reid (1978).

> Pollutant advection. The model can treat a fully three-dimensional wind field, where u, v, and w are the mean wind velocity components in the x, y, and z directions, respectively.

> Turbulent diffusion. Pollutant transport resulting from the influence of atmospheric turbulence is treated through the use of the eddy diffusivity concept. K_H and K_V are the horizontal and vertical diffusivity coefficients, respectively.

> Chemical reaction. The term R_i represents the net rate at which pollutant i is generated by chemical reactions. The reaction rate is a function of pollutant concentration, temperature, and the intensity of ultraviolet radiation.

> Emissions. The spatial and temporal distribution of the source emissions are treated in the term S_i. In the case of large point sources, the total effective plume rise is calculated to enable the appropriate spatial placement of the emissions aloft.

In addition, removal of pollutants by surface uptake processes is considered in the boundary conditions of Eq. (1).

To derive Eq. (1), one must make three assumptions. First, pollutant transport effects due to molecular diffusion are small relative to those attributable to turbulent diffusion. Second, pollutant transport due to turbulence can be adequately parameterized through the use of the eddy diffusivity concept. Third, turbulent concentration fluctuations have a negligible influence on reaction rates. For a more thorough discussion of the derivation of Eq. (1), the reader is referred to reports by Reynolds et al. (1973a, 1973b).

B. THE NUMERICAL SOLUTION PROCEDURE

Because Eq. (1) is nonlinear, it is not possible to obtain an analytical solution. Thus, one must utilize appropriate numerical techniques to find an approximate solution. To facilitate the application of finite difference methods, one first performs a change of variable to normalize the vertical dimension by the distance between the bottom and top of the region. This is accomplished by defining a new independent variable ρ as follows:

$$\rho = \frac{z - H_b(x,y,t)}{H_t(x,y,t) - H_b(x,y,t)} \quad ,$$

where H_b and H_t are the elevations of the bottom and top of the region, respectively. Upon performing this change of variable and neglecting small cross-derivative turbulent diffusion terms, Eq. (1) becomes (Reynolds et al., 1973a, 1973b):

$$\frac{\partial}{\partial t}(\Delta H c_i) + \frac{\partial}{\partial x}(u \Delta H c_i) + \frac{\partial}{\partial y}(v \Delta H c_i) + \frac{\partial}{\partial \rho}(W c_i) = \frac{\partial}{\partial x}\left(K_H \Delta H \frac{\partial c_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_H \Delta H \frac{\partial c_i}{\partial y}\right) + \frac{\partial}{\partial \rho}\left(\frac{K_V}{\Delta H} \frac{\partial c_i}{\partial \rho}\right) + R_i \Delta H + S_i \Delta H \quad , \tag{2}$$

where

$$W = w - u\left(\frac{\partial H_b}{\partial x} + \rho \frac{\partial \Delta H}{\partial x}\right) - v\left(\frac{\partial H_b}{\partial y} + \rho \frac{\partial \Delta H}{\partial y}\right) - \rho \frac{\partial \Delta H}{\partial t} \quad ,$$

$$\Delta H = H_t(x,y,t) - H_b(x,y,t)$$

As indicated in Eq. (2), the Airshed Model requires values of u, v, and W in order to carry out pollutant advection calculations. Actually, the user must specify only the values of u and v in each grid cell, and the Airshed Simulation Program computes appropriate values of W from the wind continuity relationship and information pertaining to the depth of the modeling region. To calculate W given values of u and v in each grid cell, one first writes the continuity relationship:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \tag{3}$$

Upon performing the same change of variable just described, one obtains:

$$\frac{\partial(u\Delta H)}{\partial x} + \frac{\partial(v\Delta H)}{\partial y} + \frac{\partial\overline{W}}{\partial\rho} = 0 \quad , \tag{4}$$

where

$$\overline{W} = w - u\left(\frac{\partial H_b}{\partial x} + \rho\frac{\partial\Delta H}{\partial x}\right) - v\left(\frac{\partial H_b}{\partial y} + \rho\frac{\partial\Delta H}{\partial y}\right) \quad . \tag{5}$$

The value of W used in Eq. (2) is then given by:

$$W = \overline{W} - \rho\frac{\partial\Delta H}{\partial t} \quad . \tag{6}$$

Equation (4) can be written in finite difference form and solved subject to the constraint that $\overline{W} = 0$ at the ground. Equation (6) is then used to complete the specification of the values of W employed in the numerical solution of Eq. (2).

It should be noted that reliance on this technique for assuring a mass consistent wind field should be undertaken with caution. If the u-v wind field within a layer is characterized by excessive divergence, as might occur following use of a simple interpolation scheme applied to station measurements, the divergence must be reduced by employing suitable techniques for "smoothing" the wind field prior to the simulation program. Otherwise, unrealistically large vertical velocities may result.

Special consideration must be given to the application of finite difference methods to multidimensional problems. The Airshed Model employs the so-called method of fractional steps. Applying this technique to the solution of Eq. (2), one obtains the following governing equations for the four-step numerical integration procedure:

> **Step I**

$$\frac{\partial}{\partial t}(\Delta H c_i) + \frac{\partial}{\partial x}(u \Delta H c_i) = \frac{\partial}{\partial x}\left(K_H \Delta H \frac{\partial c_i}{\partial x}\right) \quad , \qquad (7)$$

> **Step II**

$$\frac{\partial}{\partial t}(\Delta H c_i) + \frac{\partial}{\partial y}(v \Delta H c_i) = \frac{\partial}{\partial y}\left(K_H \Delta H \frac{\partial c_i}{\partial y}\right) \quad , \qquad (8)$$

> **Step III**

$$\frac{\partial}{\partial t}(\Delta H c_i) + \frac{\partial}{\partial \rho}(W c_i) = \frac{\partial}{\partial \rho}\left(\frac{K_V}{\Delta H} \frac{\partial c_i}{\partial \rho}\right) + S_i \Delta H \quad , \qquad (9)$$

> **Step IV**

$$\frac{\partial}{\partial t}(\Delta H c_i) = R_i \Delta H \quad . \qquad (10)$$

If the modeling region is divided into two layers, then there will be two sets of Eqs. (7) through (10), differing only in the definition of ΔH. The numerical integration of Eq. (2) for one time interval is approximated in the method of fractional steps by the sequential integration of Eqs. (7) through (10) for one time interval. By carrying out this four-step procedure for many time intervals, one simulates the time history of pollutant concentrations in each grid cell.

As indicated by Eqs. (7) and (8), Steps I and II of the solution procedure treat horizontal transport due to advection and diffusion. Step I integrates Eq. (7), which is transport of pollutants in the x-direction, and Step II integrates Eq. (8), transport in the y-direction. Since Steps I and II are basically the same except for the direction of integration, only Step I is discussed here. Integration of Eq. (7) is accomplished by solving the advective part of the equation:

$$\frac{\partial}{\partial t}(\Delta H c_i) + \frac{\partial}{\partial x}(u \Delta H c_i) = 0 \quad , \qquad (11)$$

using the SHASTA method developed by Boris and Book (1973). This step is described in detail by Reynolds et al. (1976). The diffusive part of Eq. (7),

$$\frac{\partial}{\partial t}(\Delta H c_i) = \frac{\partial}{\partial x}\left(K_H \Delta H \frac{\partial c_i}{\partial x}\right) \quad , \qquad (12)$$

is then solved using a standard explicit finite difference technique. The pollutant concentrations calculated in Step I are then input to Step II, which calculates the effect of transport in the y-direction.

Equations (7) and (8) cannot be solved without specifying suitable boundary conditions. At any point on the horizontal boundaries, the appropriate constraint is dependent on whether the wind is flowing into or out of the modeling region. When the wind is flowing out of the region, the partial derivative of the pollutant concentration with respect to x (Step I) or y (Step II) is set equal to zero. If the wind is flowing into the region, then the pollutant concentration must be specified along the upwind boundary.

Step III of the numerical procedure entails the integration of Eq. (9), which considers pollutant emissions and vertical advection and diffusion. The equation is solved through the use of an implicit finite difference technique to eliminate stability constraints on the size of the time step that might otherwise arise if the vertical grid spacing becomes relatively small at some point in a simulation. The computation of the vertical wind speed W is described previously by equations (4) through (6). If pollutants are advected or entrained in through the top of the modeling region, the user must specify the concentration at each species at the top of the region. Otherwise, the partial derivative of the pollutant concentration with respect to ρ is set equal to zero at the upper boundary. If the modeling region has been segmented into layers, then the resulting sets of Eq. (9) are coupled at the interface between the layers.

Integration of Eq. (10) to include the contributions of chemical reactions is the final step of the numerical procedure. A Crank-Nicolson difference scheme is employed in Step IV, which yields a set of nonlinear algebraic equations. A solution to these equations is obtained by using a Newton iterative procedure. For further discussion of the details of the finite difference equations, the reader is again referred to the reports by Reynolds et al., (1973a, 1976), and to Killus et al., (1977).

C. THE ESTIMATION OF TURBULENT DIFFUSIVITIES

Central to the treatment of turbulent diffusion processes in Eq. (2) is the estimation of the horizontal and vertical diffusivity coefficients, K_H and K_V. Because of the empirical nature of the diffusivity concept, these coefficients are difficult to measure and specify precisely. With regard to horizontal pollutant transport, advection tends to be significantly more important than turbulent diffusion processes. This dominating influence is strengthened because local concentration gradients near point and line sources cannot be represented in the Airshed Model owing to the use of a grid with relatively coarse horizontal resolution. Although the horizontal diffusion terms have a small influence on predicted concentrations, they have been retained in the model. At present, K_H is set to a constant value of 50 m^2/sec.

In contrast to horizontal transport, turbulent diffusion is frequently the dominating vertical transport process. Thus, considerable attention has been given to the development of algorithms for estimating the vertical diffusivity, K_V. The parameters used to calculate K_V are the stability class, the ground-level wind speed, the surface roughness, the height of the wind measurements, and the height of the grid cell. The first step in calculating the diffusivity is to estimate the Monin-Obukhov length. This is done by relating the Monin-Obukhov length, L, to the surface roughness, Z_0, and the stability function, S, using the following expression (Liu et al., 1976):

$$L = \frac{z_0^{(b_1 - b_2|S| + b_3S^2)}}{a_1S + a_2S^3} \tag{13}$$

where

$a_1 = 0.004349,$

$a_2 = 0.003724,$

$a_3 = 0.5034,$

$b_2 = 0.2310,$

$b_3 = 0.0325.$

This formula is a result of the best fit of observational data reported by Golder (1972). The stability function, S, a numerical representation of the Pasquill stability category, can be calculated as follows:

$$S = -\frac{1}{2}(3 - c_w + |c_e|) \cdot \mathrm{Sign}(c_e) \quad , \qquad (14)$$

where

$$\mathrm{Sign}(c_e) = \begin{cases} 1 & , \quad c_e > 0 \quad ; \\ 0 & , \quad c_e = 0 \quad ; \\ -1 & , \quad c_e < 0 \quad . \end{cases}$$

The parameters c_w and c_e are the wind speed class and exposure class respectively, and are defined as follows:

$$c_w = \begin{cases} \frac{u_r}{2} & , \quad 0 \le u_r \le 8 \text{ m/sec} \quad , \\ 4 & , \quad u_r \ge 8 \text{ m/sec} \quad ; \end{cases}$$

$$c_e = \begin{cases} 3 & , \text{ strong} \\ 2 & , \text{ moderate} \\ 1 & , \text{ slight} \end{cases} \Big\} \text{ daytime insolation ,}$$

$$\begin{cases} 0 & , \text{ heavy overcast} \quad \text{day or night ,} \\ -1 & , \ \ge\frac{4}{8} \text{ cloud cover} \\ -2 & \quad \le\frac{3}{8} \text{ cloud cover} \end{cases} \Big\} \text{ nighttime cloudiness} \quad .$$

If S = 0, the Monin-Obukhov length is set to 1.0×10^6 meters.

Next, the friction velocity, u_*, is calculated using the following equation (Liu et al., 1976):

$$u_* = \frac{ku_r}{g} \quad ,$$

where u_r denotes the wind speed measured at a reference height, z_r, and where

$$g = \begin{cases} \ln\left(\frac{z_r}{z_0}\right) + 4.7\left(\frac{z_r - z_0}{L}\right) & \text{(stable or neutral)}, \qquad (15) \\ \ln\left[\frac{1 - \phi_u\left(\frac{z_r}{L}\right)}{1 + \phi_u\left(\frac{z_r}{L}\right)}\right] - \ln\left[\frac{1 - \phi_u\left(\frac{z_0}{L}\right)}{1 + \phi_u\left(\frac{z_0}{L}\right)}\right] & \\ \quad + 2\tan^{-1}\left[\frac{1}{\phi_u\left(\frac{z_r}{L}\right)}\right] - 2\tan^{-1}\left[\frac{1}{\phi_u\left(\frac{z_0}{L}\right)}\right] & \text{(unstable)} \qquad (16) \end{cases}$$

where

$$\phi_u\left(\frac{z}{L}\right) = \left[1 - 15\left(\frac{z}{L}\right)\right]^{-1/4} \quad . \qquad (17)$$

From the calculated values of the Monin-Obukhov length and friction velocity, it is possible to calculate the vertical diffusivities for a column of cells. The method chosen to calculate the diffusivity depends on the atmospheric stability. For stable conditions, such as a cloudless night, the algorithm developed by Businger and Arya (1974) is used. The diffusivities calculated using this algorithm result in very limited vertical mixing of pollutants, as expected for stable conditions.

For neutral and unstable conditions, diffusivities are estimated by using the results of Deardorff's (1972) planetary boundary layer model to generate a theoretical concentration field downwind of a point source. Optimal control theory techniques have been employed to estimate the diffusivity profiles that cause the predicted concentration fields of Eq. (2) to agree most closely with the theoretical fields. The reader is referred to the reports by Lamb (1976), Lamb, Chen, and Seinfield (1975), and Lamb et al. (1977) for further details.

Mathematically, the algorithms used to calculate K_V can be expressed as follows:

> Stable conditions

$$K_V = \frac{k u_* z \exp\left(- \left| \frac{V_g}{u_*} \right| \frac{fz}{u_*} \right)}{1 + 4.7\left(\frac{z}{L}\right)} \quad . \tag{18}$$

> Neutral conditions

$$K_V = \frac{u_*^2}{f} \left(\alpha_0 + \alpha_1\lambda + \alpha_2\lambda^2 + \alpha_3\lambda^3 + \alpha_4\lambda^4\right) \tag{19}$$

$$\text{for } 0 < z \le 0.45 \left(\frac{u_*}{f}\right) \quad ;$$

$$K_V = 0.01 \text{ m}^2/\text{sec} \qquad \text{for } z > 0.45 \left(\frac{u_*}{f}\right) \quad . \tag{20}$$

> Unstable conditions

$$K_V = w_* z_i \Big[\beta_0 + \beta_1\zeta + \beta_2(2\zeta^2 - 1) + \beta_3(4\zeta^3 - 3\zeta) \tag{21}$$

$$+ \beta_4(8\zeta^4 - 8\zeta^2 + 1) \Big] \quad ,$$

where

$$\lambda = \frac{zf}{u_*} \quad ,$$

$$\zeta = 2\frac{z}{z_i} - 1 \quad ,$$

$$w_* = u_*\left(-\frac{1}{k}\frac{z_i}{L}\right)^{1/3} \quad ,$$

and

f = Coriolis parameter,
k = von Karman constant,
z_i = inversion height,
v_g = geostrophic wind component.

The coefficients α_i and β_i have the following values:

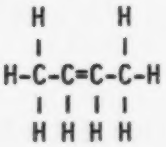
$\alpha_0 = 7.396 \times 10^{-4}$, $\beta_0 = 0.152$,
$\alpha_1 = 6.082 \times 10^{-2}$, $\beta_1 = 0.080$,
$\alpha_2 = 2.532$, $\beta_2 = -0.039$,
$\alpha_3 = -1.272 \times 10$, $\beta_3 = 0.032$,
$\alpha_4 = 1.517 \times 10$, $\beta_4 = 0.020$.

As noted earlier, the Airshed Model has the capability of including an upper layer of grid cells (frequently corresponding to the inversion layer) within the modeling region. To estimate values for K_V in this layer, vertical temperature gradient inputs are checked to establish the appropriate stability class of the layer. The corresponding equation cited above and the actual height of the grid cell is then used to calculate K_V.

D. THE TREATMENT OF ATMOSPHERIC CHEMISTRY

In the earlier discussion of Eq. (2), it was indicated that chemical effects are incorporated into the model through the term R_i, the net rate of production of pollutant i by chemical reactions. The net rate of reaction can be calculated using a chemical kinetic mechanism, which is a set of reactions and rate constants that describe the pertinent atmospheric chemical phenomena. The main chemistry mechanism employed in the Airshed Model is known as the Carbon-Bond Mechanism (CBM), as reported by Whitten and Hogo (1977) and Whitten, Hogo, and Killus (1979). A more recent version of the Carbon-Bond Mechanism (CBM II) is described in Whitten, Killus, and Hogo (1980) and Whitten, et al. (1979). The 65 reactions and rate constants in this mechanism are presented in Table A-1.

A unique feature of the Carbon-Bond Mechanism is its treatment of organic species. Since every reaction of all the organic species found in an urban atmosphere cannot be considered, these pollutants must be grouped to limit the number of reactions and species to a manageable level while permitting reasonable accuracy in predicting ozone formation. In the Carbon-Bond Mechanism, each carbon atom of an organic molecule is classified according to its bond type. For example, the carbon bonds in a butene molecule (C_4H_8) can be represented as follows:



$$\begin{array}{ccccccccccc} & & H & & & & & & H & & \\ & & | & & & & & & | & & \\ H & - & C & - & C & = & C & - & C & - & H \\ & & | & & | & & | & & | & & \\ & & H & & H & & H & & H & & \end{array}$$

This molecule has two carbon atoms associated solely with single bonds and two atoms associated with a double bond. The two carbon atoms associated with a double bond are also each associated with a single bond. In assigning

TABLE A-1. THE CARBON-BOND MECHANISM (CBM-II)
(Whitten, Killus, and Hogo, 1980)

Reaction	Rate Constant at 298°K (ppm^{-1} min^{-1})	Activation energy (K)
1. $NO_2 + h\nu \rightarrow NO + O$	Experimental	--
2. $O + O_2 + M \rightarrow O_3 + M$	$2.1 \times 10^{-5§}$	--
3. $O_3 + NO \rightarrow NO_2 + O_2$	23.9	1,450
4. $O_3 + NO_2 \rightarrow NO_3 + O_2$	4.8×10^{-2}	2,450
5. $O + NO_2 \rightarrow NO + O_2$	1.34×10^{4}	--
6. $O_3 + OH \rightarrow HO_2 + O_2$	7.7×10^{1}	1,000
7. $O_3 + HO_2 \rightarrow OH + 2O_2$	5.0	1,525
8. $NO_2 + OH \rightarrow HNO_3$	1.4×10^{4}	--
9. $CO + OH \xrightarrow{O_2} HO_2 + CO_2$	4.4×10^{2}	--
10. $NO + NO + O_2 \rightarrow 2NO_2$	$7.1 \times 10^{-10§}$	--
11. $NO_3 + NO \rightarrow 2NO_2$	2.8×10^{4}	--
12. $NO_3 + NO_2 + H_2O \rightarrow 2HNO_3$	$311 \times k\ (N_2O_5 + H_2O)^{***}$	-10,600
13. $HO_2 + NO \rightarrow NO_2 + OH$	1.2×10^{4}	--
14. $HO_2 + HO_2 \rightarrow$	1.5×10^{4}	--
15. $PAR + O \rightarrow MEO_2 + OH$	2×10^{1}	--
16. $PAR + OH \rightarrow MEO_2$	1.5×10^{3}	--
17. $OLE + O \rightarrow MEO_2 + ACO_3 + X$	2.7×10^{3}	--
18. $OLE + O \rightarrow CARB$	2.7×10^{3}	--
19. $OLE + OH \rightarrow RAO_2$	4.2×10^{4}	--
20. $OLE + O_3 \rightarrow CARB + CRIG$	8×10^{-3}	--
21. $OLE + O_3 \rightarrow CARB + MCRG$	8×10^{-3}	--
22. $ETH + O \rightarrow MEO_2 + HO_2 + CO$	6×10^{2}	--
23. $ETH + O \rightarrow CARB$	6×10^{2}	--

TABLE A-1. (Continued)

Reaction	Rate Constant at 298°K (ppm^{-1} min^{-1})	Activation energy (K)
24. $ETH + OH \rightarrow RBO_2$	1.2×10^4	--
25. $ETH + O_3 \rightarrow CARB + CRIG$	2.4×10^{-3}	--
26. $ACO_3 + NO \rightarrow NO_2 + MEO_2 + CO_2$	3.8×10^3	--
27. $RBO_2 + NO \rightarrow NO_2 + 2\ CARB + HO_2$	1.2×10^4	--
28. $RAO_2 + NO \rightarrow NO_2 + 2\ CARB + HO_2$	1.2×10^4	--
29. $MEO_2 + NO \rightarrow NO_2 + CARB + MEO_2 + X$	$(1.2 \times 10^4)(A-1)/A^{**}$	--
30. $MEO + NO \rightarrow NO_2 + CARB + HO_2$	$(1.2 \times 10^4)/A^{**}$	--
31. $MEO_2 + NO \rightarrow$ Nitrate	5×10^2	--
32. $RBO_2 + O_3 \rightarrow 2\ CARB + HO_2$	5.0	--
33. $RAO_2 + O_3 \rightarrow 2\ CARB + HO_2$	2×10^2	--
34. $MEO_2 + O_3 \rightarrow CARB + HO_2$	5.0	--
35. $CARB + OH \rightarrow \alpha(HO_2 + CO) +$ $(1 - \alpha)\ (ACO_3 + X)$	$(2.4 - \alpha) \times 10^4$	--
36. $CARB + h\nu \rightarrow CO$	$\alpha k_f^{*\ddagger\dagger}$	--
37. $CARB + h\nu \rightarrow (1 + \alpha)HO_2 +$ $(1 - \alpha)(MEO_2 + X) + CO$	$(\frac{\alpha + 1}{2})k_f^{*\ddagger\dagger}$	--
38. $X + PAR \rightarrow$	1×10^5	--
39. $ACO_3 + NO_2 \rightarrow PAN$	2×10^3	--
40. $PAN \rightarrow ACO_3 + NO_2$	$2.8 \times 10^{-2\dagger}$	12,500
41. $ACO_3 + HO_2 \rightarrow$	4×10^3	--
42, $MEO_2 + HO_2 \rightarrow$	4×10^3	--
43. $CRIG + NO \rightarrow NO_2 + CARB$	1.2×10^4	--
44. $CRIG + NO_2 \rightarrow NO_3 + CARB$	8×10^3	--
45. $CRIG + CARB \rightarrow$ Ozonide	2×10^3	--
46. $MCRG + NO \rightarrow NO_2 + CARB$	1.2×10^4	--

TABLE A-1. (Continued)

Reaction	Rate Constant at 298°K (ppm^{-1} min^{-1})	Activation energy (K)
47. MCRG + NO_2 → NO_3 + CARB	8×10^3	--
48. MCRG + CARB → Ozonide	2×10^3	--
49. CRIG → CO	6.7×10^{2}[†]	--
50. CRIG → Stable Products	2.4×10^{2}[†]	--
51. CRIG → $2HO_2$ + CO_2	9×10^{1}[†]	--
52. MCRG → Stable Products	1.5×10^{2}[†]	--
53. MCRG → MEO_2 + OH + CO	3.4×10^{2}[†]	--
54. MCRG → MEO_2 + HO_2 + CO_2	4.25×10^{2}[†]	--
55. MCRG → CARB + $2HO_2$ + CO	8.5×10^{1}[†]	--
56. ARO + OH → ARPI + ARPI + ARPI + HO_2	6×10^3	--
57. ARO + OH → HO_2 + GLY + X	1.6×10^3	--
58. ARO + OH → OH + GLY + W	1.5×10^4	--
59. W + CARB →	1.0×10^5	--
60. ARPI + NO → NO + CARB + PAR	30	--
61. ARPI + NO → NO_2 + AEROSOL	15	--
62. ARPI + NO_3 → CARB + CARB	3.5×10^4	--
63. ARPI + O_3 → AEROSOL	0.6	--
64. GLY + OH → HO_2 + ARPI + ARPI + ARPI + CO	10^4	--
65. GLY → MEO_2 + HO_2 + ARPI + ARPI + ARPI	K_{GLY}[§§]	--

---

[*] The rate constants shown are as used to model eleven experiments at UCR that used mixes of seven hydrocarbons. For that study the default values, $\alpha = 0.5$ and $A = 1.3$, were used.

[†] Units of min^{-1}.

[§] Units of $ppm^{-2}min^{-1}$.

TABLE A-1. (Concluded)

[**] A = A is the average number of $RO_2^{\cdot}$-type radicals generated from a hydrocarbon between attack by $OH^{\cdot}$ and generation of $HO_2^{\cdot}$.

[††] α is the fraction of total aldehydes that represent formaldehyde and ketones. k_f is the carbonyl photolysis rate constant.

[§§] $K_{GLY} = 0.036 \times k_{(NO_2 + h\nu)}$.

[***] $k_{(N_2O_5 + H_2O)} = 5 \times 10^{-6}$ $ppm^{-1}min^{-1}$ for UCR simulations.

carbon atoms to bond categories in the CBM, precedence is given to double bonds and carbonyl bonds. The kinetic mechanism given in Table A-1 considers five possible types of carbon bonds: single-bonded carbon atoms (PAR), very reactive double bonds (OLE), aromatic rings (ARO), carbonyl bonds (CARB), and moderately reactive double bonds (ETH). Single-bonded carbon atoms comprise not only paraffin molecules, but also portions of olefin, aromatic, aldehyde and other molecules. Double bonds are treated as pairs of carbon atoms. An activated aromatic ring is treated as a unit of six carbon atoms. The carbon atom in the carbon-oxygen double bond of an aldehyde or ketone is included in the carbonyl group. To illustrate this treatment of organic species, 1 mole of butene is considered to consist of 2 moles of single-bonded carbon atoms and 1 mole of very reactive double bonds. Table A-2 shows how other organic species are treated in the Carbon Bond Mechanism.

CBM II exhibits several important characteristics which make it suitable for incorporation in the Airshed Model. First, it has no adjustable parameters. In the formulation of CBM II, special care was taken to avoid the use of adjustable parameters that might have a profound effect on the predicted results. Other proposed mechanisms that do contain such parameters can sometimes be "tuned" to predict well for one set of conditions but must be "retuned" to fit other conditions. This limits their overall utility.

Second, CBM II was developed to be a condensation of larger, more detailed mechanisms for the reactions of propylene, butane, ethylene, toluene, formaldehyde, and acetaldehyde. Tests indicate that CBM II generates predictions that closely agree with those obtained from the more detailed mechanisms. Moreover, this correspondence was obtained without any parameter adjustments. Thus, CBM II is a condensation of present knowledge of the

TABLE A-2. CARBON-BOND PROFILES BY COMPOUND (Whitten, 1979)

SPECIES NO.	CHEMICAL NAME	OLE	PAR	ARO	CARB	ETH	UNREACTIVE
1	METHANE	0.00	0.00	0.00	0.00	0.00	1.00
2	ETHANE	0.00	0.00	0.00	0.00	0.00	2.00
3	ETHYLENE	0.00	0.00	0.00	0.00	1.00	0.00
4	PROPANE	0.00	1.50	0.00	0.00	0.00	1.50
5	PROPYLENE	1.00	1.00	0.00	0.00	0.00	0.00
6	ACETYLENE	0.00	0.00	0.00	0.00	0.00	1.00
7	CYCLOPROPANE	0.00	1.00	0.00	0.00	1.00	0.00
8	PROPADIENE	0.00	0.00	0.00	1.00	1.00	0.00
9	METHYLACETYLENE	0.00	1.50	0.00	0.00	0.00	1.50
10	*CYCLOPENTANE	0.00	3.00	0.00	0.00	1.00	0.00
11	N-BUTANE	0.00	4.00	0.00	0.00	0.00	0.00
12	BUTENE	1.00	2.00	0.00	0.00	0.00	0.00
13	ISO-BUTANE	0.00	4.00	0.00	0.00	0.00	0.00
14	1.3-BUTADIENE	1.00	0.00	0.00	2.00	0.00	0.00
15	ETHYLACETYLENE	0.00	4.00	0.00	0.00	0.00	0.00
16	N-PENTANE	0.00	5.00	0.00	0.00	0.00	0.00
17	1-PENTENE	1.00	3.00	0.00	0.00	0.00	0.00
18	2-METHYL-2-BUTENE	0.00	3.00	0.00	2.00	0.00	0.00
19	HEXANE	0.00	6.00	0.00	0.00	0.00	0.00
20	HEPTANE	0.00	7.00	0.00	0.00	0.00	0.00
21	OCTANE	0.00	8.00	0.00	0.00	0.00	0.00
22	NONANE	0.00	9.00	0.00	0.00	0.00	0.00
23	*ISOMERS OF HEXANE	0.00	6.00	0.00	0.00	0.00	0.00
24	*ISOMERS OF HEPTANE	0.00	7.00	0.00	0.00	0.00	0.00
25	N-DECANE	0.00	10.00	0.00	0.00	0.00	0.00
26	*ISOMERS OF OCTANE	0.00	8.00	0.00	0.00	0.00	0.00
27	*CYCLOHEXANE	0.00	4.00	0.00	0.00	1.00	0.00
28	UNDECANE	0.00	11.00	0.00	0.00	0.00	0.00
29	*ISOMERS OF NONANE	0.00	9.00	0.00	0.00	0.00	0.00
30	*ISOMERS OF DECANE	0.00	10.00	0.00	0.00	0.00	0.00
31	*ISOMERS OF UNDECANE	0.00	11.00	0.00	0.00	0.00	0.00
32	*N-DODECANE	0.00	12.00	0.00	0.00	0.00	0.00
33	*ISOMERS OF DODECANE	0.00	12.00	0.00	0.00	0.00	0.00
34	*N-TRIDECANE	0.00	13.00	0.00	0.00	0.00	0.00
35	*ISOMERS OF TRIDECANE	0.00	13.00	0.00	0.00	0.00	0.00
36	*N-TETRADECANE	0.00	14.00	0.00	0.00	0.00	0.00
37	*ISOMERS OF TETRADECANE	0.00	14.00	0.00	0.00	0.00	0.00
38	*N-PENTADECANE	0.00	15.00	0.00	0.00	0.00	0.00
39	*ISOMERS OF PENTADECANE	0.00	15.00	0.00	0.00	0.00	0.00
40	*C-7 CYCLOPARAFFINS	0.00	5.00	0.00	0.00	1.00	0.00
41	*C-8 CYCLOPARAFFINS	0.00	6.00	0.00	0.00	1.00	0.00
42	*C-9 CYCLOPARAFFINS	0.00	7.00	0.00	0.00	1.00	0.00
43	*TERPENES	1.00	6.00	0.00	2.00	0.00	0.00
44	*METHYLCYCLOHEXANE	0.00	5.00	0.00	0.00	1.00	0.00
45	*MINERAL SPIRITS	0.00	6.00	0.00	0.00	1.00	0.00

TABLE A-2 continued

SPECIES NO.	CHEMICAL NAME	OLE	PAR	ARO	CARB	ETH	UNREACTIVE
46	*CYCLOHEXANONE	0.00	3.00	0.00	1.00	1.00	0.00
47	*LACTOL SPIRITS	0.00	8.00	0.00	0.00	0.00	0.00
48	*ISOMERS OF BUTENE	0.00	2.00	0.00	2.00	0.00	0.00
49	*ISOMERS OF PENTENE	0.00	3.00	0.00	2.00	0.00	0.00
50	*ISOMERS OF PENTANE	0.00	5.00	0.00	0.00	0.00	0.00
51	METHYL ALCOHOL	0.00	1.00	0.00	0.00	0.00	0.00
52	ETHYL ALCOHOL	0.00	2.00	0.00	0.00	0.00	0.00
53	N-PROPYL ALCOHOL	0.00	3.00	0.00	0.00	0.00	0.00
54	ISO-PROPYL ALCOHOL	0.00	3.00	0.00	0.00	0.00	0.00
55	N-BUTYL ALCOHOL	0.00	4.00	0.00	0.00	0.00	0.00
56	ISO-BUTYL ALCOHOL	0.00	4.00	0.00	0.00	0.00	0.00
57	BUTYL CELLOSOLVE	0.00	5.00	0.00	1.00	0.00	0.00
58	TERT-BUTYL ALCOHOL	0.00	3.00	0.00	1.00	0.00	0.00
59	METHYL CELLOSOLVE	0.00	2.00	0.00	1.00	0.00	0.00
60	CELLOSOLVE	0.00	3.00	0.00	1.00	0.00	0.00
61	DIACETONE ALCOHOL	0.00	5.00	0.00	1.00	0.00	0.00
62	ETHYL ETHER	0.00	3.00	0.00	1.00	0.00	0.00
63	*GLYCOL ETHER	0.00	1.00	0.00	1.00	0.00	0.00
64	*GLYCOL	0.00	1.00	0.00	1.00	0.00	0.00
65	*PROPYLENE GLYCOL	0.00	2.00	0.00	1.00	0.00	0.00
66	ETHYLENE GLYCOL	0.00	1.00	0.00	1.00	0.00	0.00
67	TETRAHYDROFURAN	0.00	1.00	0.00	1.00	1.00	0.00
68	ACETIC ACID	0.00	2.00	0.00	0.00	0.00	0.00
69	METHYL ACETATE	0.00	0.00	0.00	0.00	0.00	3.00
70	ETHYL ACETATE	0.00	3.00	0.00	1.00	0.00	0.00
71	PROPYL ACETATE	0.00	4.00	0.00	1.00	0.00	0.00
72	N-BUTYL ACETATE	0.00	5.00	0.00	1.00	0.00	0.00
73	ETHYL ACRYLATE	0.00	2.00	0.00	1.00	1.00	0.00
74	CELLOSOLVE ACETATE	0.00	4.00	0.00	2.00	0.00	0.00
75	*ISOPROPYL ACETATE	0.00	5.00	0.00	0.00	0.00	0.00
76	*METHYL AMYL ACETATE	0.00	8.00	0.00	0.00	0.00	0.00
77	*ISOBUTYL ACETATE	0.00	6.00	0.00	0.00	0.00	0.00
78	DIMETHYL FORMAMIDE	0.00	0.00	0.00	0.00	0.00	3.00
79	*ISOBUTYL ISOBUTYRATE	0.00	7.00	0.00	1.00	0.00	0.00
80	FORMALDEHYDE	0.00	0.00	0.00	1.00	0.00	0.00
81	ACETALDEHYDE	0.00	1.00	0.00	1.00	0.00	0.00
82	*BUTYRALDEHYDE	0.00	3.00	0.00	1.00	0.00	0.00
83	ACETONE	0.00	2.00	0.00	1.00	0.00	0.00
84	METHYL ETHYL KETONE	0.00	3.00	0.00	1.00	0.00	0.00
85	METHYL N-BUTYL KETONE	0.00	5.00	0.00	1.00	0.00	0.00
86	METHYL ISOBUTYL KETONE	0.00	5.00	0.00	1.00	0.00	0.00
87	ETHYLENE OXIDE	0.00	0.00	0.00	0.00	0.00	2.00
88	*PROPYLENE OXIDE	0.00	2.00	0.00	0.00	0.00	1.00
89	ACETONITRILE	0.00	0.00	0.00	0.00	0.00	2.00
90	ACRYLONITRILE	0.00	1.00	0.00	0.00	1.00	0.00

TABLE A-2 continued

SPECIES NO.	CHEMICAL NAME	OLE	PAR	ARO	CARB	ETH	UNREACTIVE
91	ETHYLAMINE	0.00	1.00	0.00	0.00	0.00	1.00
92	TRIMETHYL AMINE	0.00	3.00	0.00	0.00	0.00	0.00
93	METHYL CHLORIDE	0.00	0.00	0.00	0.00	0.00	1.00
94	DICHLOROMETHANE	0.00	0.00	0.00	0.00	0.00	1.00
95	CHLOROFORM	0.00	0.00	0.00	0.00	0.00	1.00
96	CARBON TETRABROMIDE	0.00	0.00	0.00	0.00	0.00	1.00
97	*FREON 11	0.00	0.00	0.00	0.00	0.00	1.00
98	ETHYL CHLORIDE	0.00	0.00	0.00	0.00	0.00	2.00
99	1.1-DICHLOROETHANE	0.00	0.00	0.00	0.00	0.00	2.00
100	1.1.1-TRICHLOROETHANE	0.00	0.00	0.00	0.00	0.00	2.00
101	ETHYLENE DICHLORIDE	0.00	0.00	0.00	0.00	0.00	2.00
102	*FREON 12	0.00	0.00	0.00	0.00	0.00	1.00
103	PERCHLOROETHYLENE	0.00	2.00	0.00	0.00	0.00	0.00
104	METHYLENE BROMIDE	0.00	0.00	0.00	0.00	0.00	1.00
105	1.1.2-TRICHLOROETHANE	0.00	0.00	0.00	0.00	0.00	2.00
106	*FREON 113	0.00	0.00	0.00	0.00	0.00	2.00
107	*TRIMETHYLFLUOROSILANE	0.00	0.00	0.00	0.00	0.00	3.00
108	*MONOCHLORBENZENE	0.00	0.00	0.00	0.00	0.00	6.00
109	VINYL CHLORIDE	0.00	0.00	0.00	0.00	1.00	0.00
110	NAPTHA	0.00	8.00	0.00	0.00	0.00	0.00
111	BENZENE	0.00	0.00	0.00	0.00	0.00	6.00
112	TOLUENE	0.00	1.00	1.00	0.00	0.00	0.00
113	ETHYLBENZENE	0.00	2.00	1.00	0.00	0.00	0.00
114	1.3.5-TRIMETHYLBENZENE	0.00	3.00	1.00	0.00	0.00	0.00
115	STYRENE	0.00	0.00	1.00	0.00	1.00	0.00
116	A-METHYLSTYRENE	0.00	1.00	1.00	0.00	1.00	0.00
117	*ISOMERS OF XYLENE	0.00	2.00	1.00	0.00	0.00	0.00
118	*DIMETHYLETHYLBENZENE	0.00	4.00	1.00	0.00	0.00	0.00
119	*1.2.3-TRIMETHYLBENZENE	0.00	3.00	1.00	0.00	0.00	0.00
120	*ISOMERS OF ETHYLTOLUENE	0.00	3.00	1.00	0.00	0.00	0.00
121	*ISOMERS OF BUTYLBENZENE	0.00	4.00	1.00	0.00	0.00	0.00
122	*ISOMERS OF DIETHYLBENZENE	0.00	4.00	1.00	0.00	0.00	0.00
123	*ISOMERS OF TRIMETHYLBENZENE	0.00	3.00	1.00	0.00	0.00	0.00
124	*ISOMERS OF PROPYLBENZENE	0.00	3.00	1.00	0.00	0.00	0.00
125	PHENOLS	0.00	0.00	0.00	0.00	0.00	6.00
126	*XYLENE BASE ACIDS	0.00	2.00	1.00	0.00	0.00	0.00
127	CHLOROBENZENE	0.00	0.00	0.00	0.00	0.00	6.00
128	*1.4-DIOXANE	1.00	2.00	0.00	2.00	0.00	0.00
129	2-ETHOXYETHYL ACETATE	0.00	4.00	0.00	2.00	0.00	0.00
130	TRICHLOROETHYLENE	0.00	2.00	0.00	0.00	0.00	0.00

details of several relatively simple, yet representative, hydrocarbon systems. As future detailed studies of other organic compounds lead to a better understanding of the smog formation process, CBM II may modified to incorporate these findings.

It is well known that reaction rate constants are a function of temperature. Thus, the model treats their effects on the values of the non-photolysis reaction rate constants. In general, the atmosphere is expected to be more "reactive" on hot days than on cold days. Smog chamber experiments run at 101°F generate about 100 percent more ozone than similar experiments conducted at 61°F (Pitts et al., 1977). Given the value of a rate constant, K_r, at some reference temperature, T_r, the Arrhenius relationship for the value of k at some other temperature T can be written as:

$$k = k_r \exp\left[\frac{E_a}{R}\left(\frac{1}{T} - \frac{1}{T_r}\right)\right] \quad , \qquad (22)$$

where E_a is the activation energy of the reaction and R is the gas constant. It should be noted that the Arrhenius relationship predicts a smaller temperature effect on ozone production than that actually observed in smog chamber experiments. Thus, caution should be exercised when applying the model to situations where the ambient temperatures significantly exceed 30°C, the nominal temperature at which most smog chamber experiments are performed.

There are four photolysis reactions in the CBM, and the rate constant for each of these reactions is a function of the solar UV radiation intensity. Thus, the Airshed Model requires that the user specify the temporal variations of these rate constants. Hourly values of these parameters can be estimated from actual solar radiation measurement data using a relationship such as that proposed by Schere and Demerjian (1977).

Appreciable quantities of aerosols can cause light scattering effects that alter the intensity of UV radiation present in the atmosphere. As a result, the photolysis rate constant near the ground can be approximately 30 percent smaller than its value at the top of the modeling region when significant amounts of aerosol are present. Using predictions of aerosol concentrations in a column of grid cells, the model estimates the rate constants at the bottom and top of the modeling region. The values at intermediate points are estimated by linear interpolations. This is described further in Killus, et al. (1977).

E. THE TREATMENT OF EMISSIONS

The Airshed Model can accommodate emissions both at the ground and aloft. The emissions from a particular source are injected into the appropriate grid cell. Because of the finite resolution of the model, these emissions are mixed instantaneously throughout the cell. The magnitude and spatial and temporal distribution of emissions must be specified for all pollutants being simulated in the model. Furthermore, emissions of organic compounds must be grouped according to the carbon-bond categories discussed previously. This step can be accomplished through the use of available emissions composition measurements or the results of other studies carried out in similar urban areas. An example of one such study for Los Angeles is reported by Trijonis and Arledge (1976). A large organic species data base is reported by Bucon, Macko, and Taback (1978), also based on Los Angeles.

Such data can be readily used to apportion hydrocarbon emissions to the five carbon-bond categories. The basic approach is to first compute the number of moles of each organic species emitted by a given source as follows:

$$Q_{m_i} = \left(\frac{X_i Q}{100}\right)/M_i$$

where Q = total hydrocarbons emitted (grams)
X_i = weight percent of species i in emissions Q
M_i = molecular weight of species i (grams)
Q_{m_i} = moles of species i emitted (gram-moles)

One then uses the carbon-bond profiles by species given in Table A-2 to compute the number of moles of each carbon-bond associated with each organic species. For example, if a source emits 120 moles (Q_{m_i}) of cyclohexane (entry 27 in Table A-2), this is equivalent to emitting 480 moles of single-bonded carbon atoms (PAR) and 120 moles of moderately reactive double bonds (ETH).* Once the number of moles of carbon-bonds has been computed for each species, the results can be summed to compute the total number of moles of each carbon-bond emitted by the source.

The overall procedure is illustrated in Table A-3. In this example, the weight percents were obtained from Bucon, Macko, and Taback (1978) and are representative of architectural surface coating emissions, primarily trade paints. The computations indicate that for every 100 grams of hydrocarbons emitted, there are 4.66 gram-moles of single-bonded carbon atoms (PAR), 0.121 gram-moles of aromatic rings (ARO), 0.25 gram-moles of carbonyl bonds (CARB), and 0.25 gram-moles of moderately reactive double bonds (ETH). To obtain the

*Note that the ring structure of cycloparaffins is more photochemically reactive than straight chain paraffins. The opening of the ring structure is treated as if the ring is a moderately reactive double bond.

TABLE A-3. EXAMPLE COMPUTATION OF THE EMISSIONS OF THE FIVE CARBON-BONDS FOR AN INDIVIDUAL SOURCE

SPECIES	Molecular Weight (grams)	Weight Percent (%)	Compound (moles)	OLE (moles)	PAR (moles)	ARO (moles)	CARB (moles)	ETH (moles)
N-Hexane	86.2	20.7	0.240	-	1.440	-	-	-
Cyclohexane	84.2	20.7	0.246	-	0.984	-	-	0.246
Isomers of Xylene	106.2	2.6	0.024	-	0.048	0.024	-	-
Toluene	92.1	5.2	0.056	-	0.056	0.056	-	-
Ethyl Benzene	106.2	4.3	0.041	-	0.082	0.041	-	-
Acetone	58.1	3.2	0.055	-	0.110	-	0.055	-
Methyl Ethyl Ketone	72.1	5.6	0.078	-	0.234	-	0.078	-
Methyl N-Butyl Ketone	100.2	0.7	0.007	-	0.035	-	0.007	-
Methyl Isobutyl Ketone	100.2	0.6	0.006	-	0.030	-	0.006	-
Methyl Alcohol	32.0	3.9	0.122	-	0.122	-	-	-
Ethyl Alcohol	46.1	0.6	0.013	-	0.026	-	-	-
Isopropyl Alcohol	60.1	16.4	0.273	-	0.819	-	-	-
N-Butyl Alcohol	74.1	1.6	0.022	-	0.088	-	-	-
Isobutyl Alcohol	74.1	0.6	0.008	-	0.032	-	-	-
Propylene Glycol	76.0	0.8	0.011	-	0.022	-	0.011	-
Ethylene Glycol	62.1	0.6	0.010	-	0.010	-	0.010	-
N-Butyl Acetate	116.2	2.5	0.022	-	0.110	-	0.022	-
Isobutyl Acetate	116.2	1.5	0.013	-	0.078	-	-	-
Dimethyl Formamide	73.1	0.5	0.007	-	-	-	-	-
Isobutyl Isobutyrate	144.2	6.1	0.042	-	0.294	-	0.042	-
2-Ethoxyethyl Acetate	132.0	1.3	0.010	-	0.040	-	0.020	-
TOTAL				-	4.660	0.121	0.251	0.246
				x 28	x 14	x 78	x 30	x 28
WEIGHT PERCENTS				-	65.2	9.4	7.5	6.9

corresponding weight percent of each carbon-bond, the number of gram-moles is multiplied by the weight of the carbon-bond unit. These weights are as follows:

PAR	@ CH_2	14 grams
OLE	@ C_2H_4	28 grams
ETH	@ C_2H_4	28 grams
ARO	@ C_6H_6	78 grams
CARB	@ COH_2	30 grams

In this example, the carbon-bond weight percents are therefore 65.2% PAR, 9.4% ARO, 7.5% CARB, and 6.9% ETH. Once such a profile of carbon-bond weight percents is developed, it can be readily applied to an emission rate Q to obtain the number of moles for each carbon-bond as follows:

$$PAR = \left(\frac{\text{wt \% PAR}}{100}\right) Q/14$$

$$OLE = \left(\frac{\text{wt \% OLE}}{100}\right) Q/28$$

$$ETH = \left(\frac{\text{wt \% ETH}}{100}\right) Q/28$$

$$ARO = \left(\frac{\text{wt \% ARO}}{100}\right) Q/78$$

$$CARB = \left(\frac{\text{wt \% CARB}}{100}\right) Q/30.$$

Emissions released at or near ground level are injected into the lowest level of grid cells. Emissions emanating from elevated point sources are injected into the appropriate grid cell corresponding to the total effective plume rise, Δh_p:

$$\Delta h_p = \Delta h_s + \Delta h_\infty ,$$

where Δh_s is the stack height and Δh_∞ is the ultimate plume rise relative to the top of the stack. To estimate Δh_∞, the following algorithms recommended by Briggs (1971) are employed:

> When s > 0 and u ≥ 1 m/sec,

$$\Delta h_\infty = 8.7 \left(\frac{Q}{us}\right)^{1/3} \quad . \tag{23}$$

> When s > 0 and u ≤ 1 m/sec and when Δh_∞ is less than Δh_∞ predicted by Eq. (23),

$$\Delta h_\infty = 8.6\ Q^{1/4}\ s^{-3/8} \quad . \tag{24}$$

> When s < 0 and Q ≥ 20 MW,

$$\Delta h_\infty = 15.3\ Q^{1/3}\ \Delta h_s^{2/3}\ u^{-1} \quad . \tag{25}$$

> When s ≤ 0 and Q < 20 MW,

$$\Delta h_\infty = 20.8\ Q^{1/3}\ X^{2/3}\ u^{-1} \quad . \tag{26}$$

In Eqs. (23) through (26),

$$s = \left(\frac{g}{T}\right)\left(\frac{\partial\theta}{\partial z}\right) \quad ,$$

$$X = Q^{2/5} \Delta h_s^{3/5} \quad ,$$

and

Q = rate of heat emissions (MW),
u = wind speed at height Δh_s (m/sec),
g = gravitational acceleration (m/sec^2),
T = mean ambient temperature (°K),
θ = potential temperature (°K).

The problem of plume penetration into or through stable layers aloft (temperature inversions) is also important. Normally this is handled by comparing the potential temperature of the plume at some elevation with that of the ambient air at the same elevation (Briggs, 1971). The plume should continue to rise as long as its potential temperature is higher. Therefore, to determine the fate of the plume when it encounters a temperature inversion, provisions have been made in the Airshed Model to compute the difference between the plume and ambient potential temperatures, $\Delta\theta$, using relationships suggested by Briggs (1971). If $\Delta\theta$ is predicted to be greater than zero at the base of the inversion, then the plume is allowed to rise until the point where $\Delta\theta = 0$ is reached. If the plume rises higher than the top of the modeling region, then the pollutants carried in the plume are excluded from subsequent Airshed Model calculations.

F. THE TREATMENT OF SURFACE UPTAKE

Pollutant removal processes are incorporated into the Airshed Model through the use of the deposition velocity concept, that is, the uptake flux of pollutant i at the surface, F_{di}, is proportional to the ground-level concentration C_{gi}. The proportionality constant is the effective deposition velocity, V_{di}. Mathematically, the flux can be written as follows:

$$F_{di} = V_{di} C_{gi} \tag{27}$$

The uptake of a pollutant takes place in three sequential stages:

> Transport to just above the surface by advection and turbulent diffusion.

> Transport to the surface itself by processes that are influenced by the shape of the surface.

> Absorption, adsorption, or chemical reaction at the surface.

Thus, the overall removal rate is affected by both transport and chemical processes.

To estimate values for V_{di}, one applies the concept of a resistance to transport, R_t, and to surface removal, R_{si}. One then defines V_{di} as follows:

$$V_{di} = \frac{1}{R_t + R_{si}} . \qquad (28)$$

When either resistance is large, V_{di} approaches zero.

To parameterize the transport resistance, the results of studies carried out by Owen and Thompson (1963) and Chamberlain (1966) are employed to obtain:

$$R_t = u_r u_*^{-2} + B^{-1} u_*^{-1} , \qquad (29)$$

where u_r is the wind speed at a reference height of 10 meters, and B^{-1} is an empirically determined function having the following value:

$$B^{-1} = 2.2 \, u_*^{-1/3} . \qquad (30)$$

The surface resistance R_{si}, is dependent on the pollutant and on the type of surface. To determine the surface resistance for grid square j, R_{sij}, one calculates the average surface uptake velocity $V_{sij} = \left(R_{sij}^{-1}\right)$ from:

$$V_{sij} = \sum_k \alpha_{jk} \beta_k V_{si}^r , \qquad (31)$$

where

$\alpha_j k$ = fraction of grid square j represented by land use k,

β_k = a factor that adjusts the reference surface uptake velocity to that for land use k,

V_{si}^r = reference surface uptake velocity for pollutant i.

Values of β_k for central business district, suburban residential, and rural/agricultural land use categories have been estimated at 0.2, 0.5, and 1.0, respectively (Killus et al., 1977). To satisfy the input requirements of the Airshed Model, the user must estimate values of

$$\sum_k \alpha_{jk}\beta_k$$

for each ground-level grid cell in the modeling region. Further information pertaining to the parameterization of pollutant removal processes, is found in Killus et al., (1977).

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